

- I. On a Family of Generalized Colorings
- II. Some Contributions to the Theory of
Neural Networks.
- III. Embeddings of Ultrametric Spaces.

Thesis by
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"The operations of logic will have to be treated by procedures which allow exceptions with low but non-zero probabilities ... This new system of formal logic will move closer to another discipline which has been little linked in the past with logic. This is thermodynamics ... "

John Von Neumann

(Hixon Symposium, Caltech September 1948)

To Ezio and Jose.

Acknowledgements

The three years I have spent at Caltech have been among the happiest, and in this regard I am indebted to the whole community for providing me with such an outstanding environment.

I happen to be interested in polynomial time algorithms. However, the list of persons I should acknowledge has been growing exponentially over time. I could not omit:

- Richard Wilson, my advisor, for his intellectual honesty, patience, open-mindedness and precious insight

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Introduction

This thesis comprises three apparently very independent parts. However, there is a unity behind I would like to sketch very briefly.

Formally graphs are in the background of most chapters and so is the duality local versus global. The first section is concerned with globally coloring graphs under some local assumptions. Algorithmically it is an intrinsically difficult task and neural networks, the topic of the second part can be used to approach intractable problems. Simple local interactions with emergent collective behavior are one of the essential features of these networks. Their current models are similar to some of those encountered in statistical mechanics, like spin glasses. In the third part, we study ultrametricity, a concept recently rediscovered by theoretical physicists in the analysis of spin-glasses. Ultrametricity can be expressed as a local constraint on the shape of each triangle of the given metric space.

Unless otherwise stated, results in the first and second part are essentially original. Since the third part represents a joint work with Michael Aschbacher, Eric Baum and Richard Wilson, I should perhaps try to outline my contribution though paternity of collective results is somewhat fuzzy. While working on neural networks and spin glasses Eric and I got interested in ultrametricity. Several of us had found an initial polynomial upper bound, but the final results of " $n + 1$ " was first reached independently by Michael and Richard. I think I obtained the theorems: 4.5, 6.1, 6.3 (using an idea of Eric), 6.4, 6.5, 6.6, 6.7 (with Richard and helpful references from Bruce Rothschild and Olga Taussky) and participated in some other results.

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ON A FAMILY OF GENERALIZED COLORINGS

Abstract--Motivated by a question in cellular telecommunication technology, we investigate a family of graph coloring problems where several colors can be assigned to each vertex and no two colors are the same within any ball of radius R . We find bounds and coloring algorithms for several kinds of graphs. We introduce possible conjectures with implications for the four color theorem and show some partial results.

I. INTRODUCTION

The following problem was suggested to me by E. C. Posner and has its origins in cellular telecommunication technology. The two basic concepts of cellular radio are: cell splitting and frequency reuse. Very schematically: in order to provide a flexible, large scale, low cost mobile telephone service to a given area using a limited band in the radio spectrum, the strategy that has been adopted consists in dividing the area into "cells". When a call is originated in a cell, a radio frequency is allocated to the call. The same frequency can be used at the same time in another cell, provided the distance between the two cells is greater than a certain value to avoid possible interferences. The cells are therefore grouped into clusters. At any time, all the frequencies being used within one cluster need to be distinct. For reasons of economy, scaling and systematization, designers have generally adopted a tiling of the service area using hexagonal cells. The following formalization can be made.

Let $G = (V,E)$ be a graph (the vertices V correspond to

the cells and the edges E connect neighboring cells) with the metric induced by the shortest path between points. Let $f: V \rightarrow \mathbb{N}$ be the call function, i.e. $f(x)$ is the total number of calls in cell x . Let R be a fixed positive radius. The call coloring problem on G consists in assigning $f(x)$ colors (frequencies) to each vertex x in V with the constraint that within any ball $B(x,R)$ of radius R , all colors be different. The corresponding call chromatic number will be denoted by: $C_R^f(G)$. Often, to be more specific, we shall need some assumptions on f . Two cases are of particular interest:

1st case: When $f(x) = k = \text{cst}$. We shall write:

$C_R^{f=k}(G)$ or $C_R^k(G)$ for the constant call chromatic number

2nd case: When $\sum_{x \in B(y,R)} f(x) \leq K$ for a fixed constant

K and any ball $B(y,R)$. Such an f will be said to be K admissible with radius R and $\mathcal{F}_{R,K}(G)$ is the class of all such functions on G . Without loss of generality we shall always assume that the bound K is attained in at least one ball. The bounded call coloring number will be denoted: $C_{R,K}^f(G)$. We shall be particularly interested in:

$$C_{R,K}(G) = \max_{\mathcal{F}_{R,K}} C_{R,K}^f(G)$$

How does $C_{R,K}(G)$ behave as a function of R, K and G ? Trivially $C_{R,K}(G) \geq K$ and if $R = 0$ or $R = \infty$ then $C_{R,K}(G) = K$. Are these limit cases significative?

It should be noticed that both $C_R^{f=k}(G)$ and $C_R^f(G)$ can be written as $C_{R,K}^f(G)$ for the appropriate choice of K . Also, in

view of possible applications to cellular radio we are interested in finding $C_{R,K}(T.L.)$ where T.L. denotes the triangular lattice corresponding to the dual of the hexagonal tiling. From now on, without loss of generality, we shall assume that G is simple (no loops, no multiple edges) and connected. We shall use the notations $d(x)$ for the degree of any x in V , $\Delta(G)$ for the maximum degree and K_n for the complete graph on n vertices. Two vertices x and y will be said to "interact" iff they are contained in a same ball of radius R i.e. iff $d(x,y) \leq 2R$.

II. RELATION TO CHROMATIC NUMBER

SIMPLE BOUNDS AND FIRST PROPERTIES

Let us briefly explore the relations between the usual chromatic number $C(G)$ of a graph G and the call chromatic number.

Proposition 2.1:

For any graph G and any integer radius R we can construct a graph $S_R(G)$ and a call function f in $\mathcal{F}_{R,2}$ such that:

$$C(G) = C_R^f(S_R(G)) .$$

Proof: Define $S_R(G)$ and f by inserting $2R - 1$ vertices on each original edge of G and by setting f to 1 on the original vertices of G and to 0 on the newly created vertices. Call colorings of $S_R(G)$ are then in one to one correspondence with traditional colorings of G .

Call coloring appears as a generalization of usual coloring and therefore it is at least as difficult. In particular it is NP complete. Yet the reduction is also possible in the other direction.

Proposition 2.2:

For any graph G , any integer radius R and any call function f , we can construct a graph $\psi_R^f(G)$ such that:

$$C_R^f(G) = C(\psi_R^f(G)) .$$

Proof: Description of the operation ψ_R^f :

- (1) Replace each vertex x of G for which $f(x) \neq 0$ by a

complete graph $K_{f(x)}$ on $f(x)$ points

(2) If a is in the clique $K_{f(x)}$ and b is in the clique $K_{f(y)}$ then draw an edge (a,b) iff x and y interact in G i.e. iff $d(x,y) \leq 2R$.

(3) Delete all vertices and incident edges corresponding to original vertices x in G for which $f(x) = 0$. It is essential to delete these points only at the end of the process since they may still play a role in (2) by being on a path of length less or equal to $2R$ connecting two vertices of G . We leave as an easy exercise to check that $\psi_R^f(G)$ has the required properties.

As in the case of the usual chromatic number $C(G)$, we can, by using a weaker version of Zorn's lemma (like the compactness theorem in logic or the prime ideal theorem on boolean algebras) restrict ourselves to the case where G is finite. Indeed if $C_{R,K}(G') \leq C$ for any finite subgraph G' of G then: $C_{R,K}(G) \leq C$.

Using a well known property of $C(G)$ we get:

Proposition 2.3:

$$C_R^f(G) \leq \Delta (\psi_R^f(G)) + 1$$

More generally, all known bounds on the chromatic number can be applied to $\psi_R^f(G)$ in order to get a bound on the call chromatic number. For instance, we could use the map color theorem of Heawood. Yet for this purpose the genus of $\psi_R(G)$ should be known, and this is in general very delicate. If

$\psi_R^f(G)$ is planar, then 4 colors suffice. Yet if G contains a vertex x with $f(x) \geq 5$ then $\psi_R^f(G)$ will contain a K_5 and therefore will not be planar. We can also restate Proposition 2.3 in terms of the graph G only:

Proposition 2.4:

$$C_R^f(G) \leq \max_{\substack{x_0 \in V(G) \\ f(x_0) \neq 0}} \left[\sum_{x \in B(x_0, 2R)} f(x) \right]$$

This is because, by construction on ψ_R^f , we have:

$$1 + \Delta(\psi_R^f(G)) = \max_{\substack{x_0 \in V(G) \\ f(x_0) \neq 0}} \left[\sum_{x \in B(x_0, 2R)} f(x) \right]$$

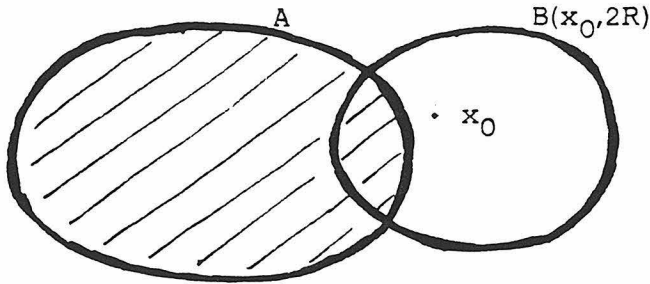
So, if the total number of calls in a ball of radius $2R$ is bounded by a constant L , then L colors suffice for the call coloring problem. If G has a regular structure and is embedded in an euclidean space of dimensions d , then we get an inequality of the type:

$$K \leq C_{R,K}(G) \leq n(d) K$$

where $n(d)$ is the minimum number of balls of radius R needed to cover entirely a ball of radius $2R$. Therefore for general regular structures we can already expect a linear upper bound in K .

We shall attempt now a careful study of the call coloring problem for several particular graphs. In many instances we shall use an inductive coloring procedure. Assume that $G =$

(V,E) , R , K , and f in $\mathcal{F}_{R,K}(G)$ are given. Let A be a subset of V and x_0 a vertex of $V - A$. Assume that A has already been call colored using m colors. We want to extend the coloring to x_0 . Let $A(x_0) = A \cap B(x_0, 2R)$. As far as extending the coloring, x_0 interacts only with points in $A(x_0)$.



Therefore if $m \geq f(x_0) + \sum_{x \in A(x_0)} f(x)$

we can call color $A \cup \{x_0\}$ with m colors. In particular we have the basic extension lemma:

Lemma 2.5:

Let G , R , K and f in $\mathcal{F}_{R,K}$ be given.

Let $A \subset V(G)$ and $x_0 \in V - A$.

Let $A(x_0) = A \cap B(x_0, 2R)$

Let $m \geq K$ and assume A has been call colored with m colors.

Then if we can find a vertex $y_0 \in V(G)$ such that:

$$B(y_0, R) \supset A(x_0) \cup \{x_0\}$$

the m call coloring of A can be extended to $A \cup \{x_0\}$.

Proof: Since $A(x_0) \cup \{x_0\}$ is in $B(y_0, R)$ we have, by K admissibility of f :

$$\sum_{x \in A(x_0)} f(x) + f(x_0) \leq K \leq m .$$

Successive applications of the extension lemma can yield a coloring algorithm at least for certain subsets of $V(G)$.

As a function of f , R , K and G , $C_{R,K}^f(G)$ has many simple trivial properties. Some of them appear in the next lemma.

Lemma 2.6:

- (1) $C_R^{mf}(G) \leq m C_R^f(G)$ for $m \geq 0$
- (2) $C_R^{f_1+f_2}(G) \leq C_R^{f_1}(G) + C_R^{f_2}(G)$
- (3) $C_R^f(G) \leq C_{R'}^f(G)$ for $R \leq R'$

We now estimate $C_{R,K}^f(G)$ for several basic graphs G .

III. LINEAR PATHS, TREES AND N-GONES:

(1) Linear Path P:

By linear path we refer to the graph



Proposition 3.1:

For any K, R , linear path P and f in $\mathcal{F}_{K,R}(P)$:

$$C_{R,K}^f(P) = K$$

Proof: By induction and using the extension lemma at each step or as a special case of the next theorem. It should be noticed that the coloring algorithm is very simple: start from one end and use the colors $1, 2, \dots, K$ cyclically in sequence.

(2) Tree T:

Theorem 3.2:

For any K, R , tree T and f in $\mathcal{F}_{K,R}(T)$:

$$C_{R,K}^f(T) = K$$

Proof: Root the tree T at a vertex α and color $B(\alpha, R)$ with K colors. Now partition the remaining vertices into classes L_1, L_2, \dots where $L_i = \{x \in V(T) : d(x, \alpha) = R+i\}$. Define $g(i) = |L_i|$. We are going to color the levels L_i in succession using the extension lemma. Assume that $L_{i+1} = \{x_1, \dots, x_{g(i+1)}\}$ and that

L_1, L_2, \dots, L_i and $\{x_1, \dots, x_j\}$ have already been call colored. To color x_{j+1} notice there is a unique path joining x_{j+1} to α and it has length $R + i + 1$. Let y_0 be the unique point on this path such that $d(y_0, x_{j+1}) = R$. We then apply the lemma with:

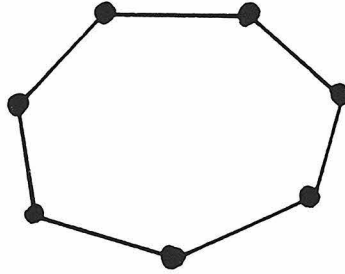
$A = B(\alpha, R) \cup L_1 \cup \dots \cup L_i \cup \{x_1, \dots, x_j\}$, y_0 and $x_0 = x_{j+1}$. It is easy to check that:

$$B(y_0, R) \supset \{x_0\} \text{ and}$$

$$B(y_0, R) \supset A(x_0)$$

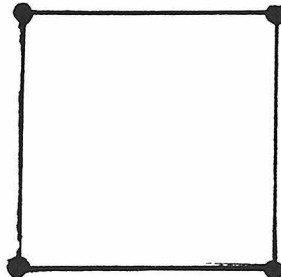
(3) N-gone G_N

By N-gone we mean the graph of length N:



We obviously have: $K \leq C_{R,K}^f \leq 2K$ since we can subdivide G_N into two linear paths P_1 and P_2 and use two sets of K colors, one for each path by Proposition 3.1. Remark also that if $f = k = \text{cst}$ then $K = (2R+1)k$ (at least as soon as $N \geq 2R+1$). If we look at the case: $N = 4$ $R = 1$ $f = 1$ we have $K = 3$ and it is easy to see that $C_{1,3}^{f=1}(G_4) = 4 > 3$. This is the first example we encounter where the lower bound can be violated.

$$C_{1,3}^{f=1} = 4$$



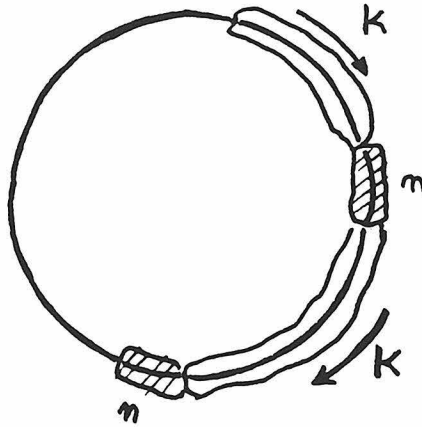
$$f = 1$$

$$R = 1$$

$$N = 1$$

$$K = 3$$

A complete study of the case $f = k$ seems to be necessary. Given any two vertices x and y of G_N , K colors can be used to color one of the linear paths from x to y . Conflicts could arise only if $d(x,y) \leq 2R$ along the other path. This suggests the idea of using K colors for the main path and a set of n additional colors for the vertices on the other path. We can even try to use the n colors in some "evenly" distributed regions of the N -gone and the other K colors cyclically in sequence between these regions, as in the figure.



Along any path between two points the colors $1, \dots, K$ are used cyclically with perhaps some insertions of colors belonging to the n additional colors. Therefore as in Proposition 3.1 no conflict can arise along such a path. The problem is therefore to find how to minimize n . It is important to notice that if v_0, v_1, \dots, v_s is a maximal sequence of consecutive vertices where the n -colors are used then not all the calls corresponding to v_0 and v_s need to be colored using some of the n -colors. Colors in $\{1, \dots, K\}$ can be used, provided they agree with the global cyclical use of these colors on G_N .

More formally:

Proposition 3.3: Let R, K, N be fixed and f in $\mathcal{F}_{R,K}(G_N)$. Fix

an orientation for G_N and assume that a set $S = \{x_0, \dots, x_{2m-1}\}$ of $2m$ distinct vertices of G_N has been selected. Let I_i be the set of vertices strictly in between x_i and x_{i+1} (for any i and mod. $2m$). Let a and b be two integer functions on S such that: $a(x_i) + b(x_i) = f(x_i)$ $i = 0, \dots, 2m-1$. Assume that:

(i) the calls corresponding to: I_{2j} $j = 0, \dots, m-1$ and $a(x_i)$ $i = 0, \dots, 2m$ have been colored using a set of n colors.

$$(ii) \sum_{i=0}^{2m-1} b(x_i) + \sum_{j=0}^{m-1} \sum_{x \in I_{2j+1}} f(x) \equiv 0 \pmod{K}$$

Then $C_{R,K}(G_N) \leq K + n$ and the colors $\{1, \dots, K\}$ can be used cyclically to complete the partial coloring of (i).

Proof: Use the colors $\{1, \dots, K\}$ in order and cyclically on the calls corresponding to $b(x_i)$ and to the I_{2j+1} . By assumption (i) conflicts could arise only between two such calls. But this is in contradiction with Proposition 3.1 and our previous remarks. We have the easy corollaries:

Corollary 3.4:

$$\text{If } \sum_{x \in V(G_N)} f(x) \equiv 0 \pmod{K} \text{ then:}$$

$$C_{R,K}^f(G_N) = K$$

Corollary 3.5:

If $f(x) = k = \text{cst.}$ then the following are equivalent:

$$a) C_R^k(G_N) = K$$

$$b) \sum_{x \in V(G_N)} f(x) \equiv 0 \pmod{K}$$

$$c) N \equiv 0 \pmod{2R+1}$$

Therefore if $N \not\equiv 0 \pmod{2R+1}$

$$C_R^k(G_N) > K.$$

We can now completely solve the regular case.

Theorem 3.6

For any k and R , if $N = a + b(2R+1)$ with $0 \leq a \leq 2R$ and $0 \leq b$ then:

$$C_R^k(G_N) = \begin{cases} kN & \text{for } b = 0, 1 \\ (2R+1)k + \left\lceil \frac{ka}{b} \right\rceil & \text{for } b \geq 2. \end{cases}$$

($\lceil t \rceil = \max \{u \in \mathbb{Z}, t \leq u\}$)

Proof: Use Proposition 3.3 with $K = (2R+1)k$, $n = \left\lceil \frac{ka}{b} \right\rceil$ and $m = b$. Notice that we have:

$$\sum_{x \in I_{2j+1}} f(x) = K \quad j = 0, \dots, b-1$$

If $x \in I_{2i}$ and $y \in I_{2i+2}$, the number of calls between x and y is at least K and therefore $d(x,y) > 2R$ and there is no problem in coloring x and y using the n additional colors because:

$$\begin{aligned} \sum_{x \in V(G_N)} f(x) &= kN = ka + kb(2R+1) \\ &\leq bn + bk. \end{aligned}$$

Therefore $C_R^k(G_N) \leq (2R+1)k + \left\lceil \frac{ka}{b} \right\rceil$

If a is zero, then we know by Corollary 3.5 that $C_R^k(G_N) = k$. Also if $a \neq 0$ and $b > ka$, then $K < C_R^k(G_N) \leq K + 1$ and again the formula is exact. If $1 \leq N \leq 4R + 1$ then any two vertices interact and all colors need to be different. Therefore

$$C_R^k(G_N) = kN \quad \text{for } 1 \leq N \leq 4R + 1$$

Finally the only open cases left are:

$$N = a + b(2R+1) \quad \text{with } 0 < a \leq 2R \quad \text{and} \quad 1 < b \leq ka .$$

Assume for contradiction that:

$$C_R^k(G_N) \leq k(2R+1) + \left\lceil \frac{ka}{b} \right\rceil - 1 . \quad \text{Then:}$$

$$b(k + \left\lceil \frac{ka}{b} \right\rceil - 1) < kN \leq (b+1)(k + \left\lceil \frac{ka}{b} \right\rceil - 1) .$$

So, at least one of the colors must have been used at least $b + 1$ times. The distance between any two reuses must be at least $2R + 1$ to avoid interference. Therefore we must have: $(b+1)(2R+1) \leq N$. But by assumption, $N \leq 2R + b(2R+1)$ which yields a contradiction.

Next we have two tables with several values of $C_R^k(G_N)$.

R = 1					
N \ k	1	2	3	4	5
1	1	2	3	4	5
2	2	4	6	8	10
3	3	6	9	12	15
4	4	8	12	16	20
5	4	10	15	20	25
6	3	6	9	12	15
7	4	7	11	14	18
8	4	8	12	16	20
9	3	6	9	12	15
10	4	7	10	14	17
11	4	8	12	15	19
12	3	6	9	12	15
13	4	7	10	13	17
14	4	7	11	14	18
15	3	6	9	12	15
16	4	7	10	13	16
17	4	7	11	14	17
18	3	6	9	12	15
19	4	7	10	13	16
20	4	7	10	14	17
21	3	6	9	12	15
22	4	7	10	13	16
23	4	7	10	14	17
24	3	6	9	12	15
25	4	7	10	13	16

a = 1 b = 2

a = 2

a = 1 b = 3

a = 2

a = 1 b = 4

a = 2

a = 1 b = 5

a = 2

a = 1 b = 6

a = 2

a = 1 b = 7

a = 2

Table of $C_{R=1}^k(G_N)$

R = 2			
N \ k	1	2	3
1	1	2	3
2	2	4	6
3	3	6	9
4	4	8	12
5	5	10	15
6	6	12	18
7	7	14	21
8	8	16	24
9	9	18	27
10	5	10	15
11	6	11	17
12	6	12	18
13	7	13	20
14	7	14	21
15	5	10	15
16	6	11	17
17	6	12	17
18	6	12	18
19	7	13	19
20	5	10	15
21	6	11	16
22	6	11	17
23	6	12	18
24	6	12	18
25	5	10	15

a = 1 b = 2

a = 2 "

a = 3 "

a = 4 "

a = 1 b = 3

a = 2 "

a = 2 "

a = 4 "

a = 1 b = 4

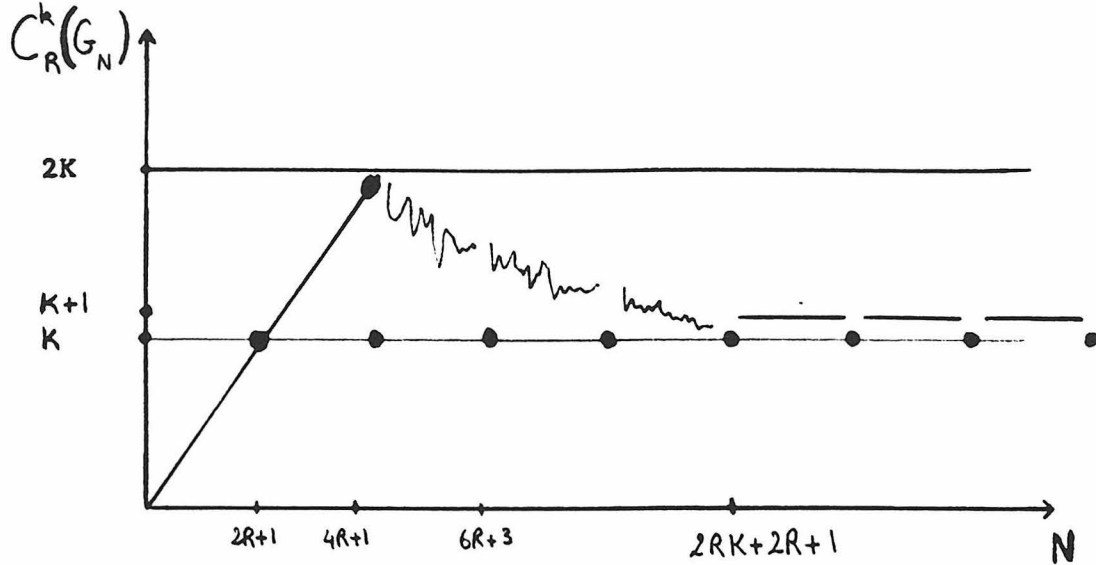
a = 2 "

a = 3 "

a = 4 "

Table of $C_{R=2}^k(G_N)$

The interesting behavior of C_R^k can be summarized in the following graph.



The case where f is periodic can also be treated in detail. However for a general f precise values of $C_{R,K}^f$ will depend on f . We only know that $K \leq C_{R,K}^f(G_N) \leq 2K$. Yet the natural question to ask is: for N large enough do we have:

$K \leq C_{R,K}^f(G_N) \leq K + 1$? This is indeed the case.

Theorem 3.7:

Let K, R be fixed. For $N \geq (4R+1)(K-1)$ and for any f in $\mathcal{F}_{R,K}(G_N)$ we have:

$$K \leq C_{R,K}^f(G_N) \leq K + 1.$$

Proof: Let $\sum_{x \in V(G_N)} f(x) \equiv c \pmod{K}$. If $c = 0$ we have seen

that K colors are enough. Otherwise the largest possible value for c is $K - 1$. Therefore, to use $K + 1$ colors at most, we must be able to select in the worst case $K - 1$ single calls of G_N , separated by a distance of at least $2R + 1$, and use a unique color for these calls. The remaining calls are a

multiple of K and can therefore be colored using the colors $\{1, \dots, K\}$ cyclically. If f is zero on $2R + 1$ consecutive vertices we can use K colors in sequence on the remaining vertices. Therefore we can assume that f is never zero on $2R + 1$ consecutive vertices. So, the distance between any two consecutive calls where the additional color is used is at most $2R + 2R + 1 = 4R + 1$. There are at most $K - 1$ such calls. Therefore if $N \geq (4R+1)(K-1)$ $C_{R,K}^f(G_N) \leq K + 1$. This bound on N is very crude and can be improved. In the regular case, as soon as $N \leq 2R(K+1)$ $K + 1$ colors always suffice. Our complete knowledge of $C_R^K(G_N)$ will be useful in the study of other graphs. Interesting lower bounds can be obtained using the "abnormal" behavior of $C_R^K(G_N)$ for cycles of small length. As an example, if a graph G contains a G_{32} and if $K = 33$ and $R = 5$, then since $C_5^3(G_{32}) = 33 + 15 = 48$ we have: $C_{5,33}(G) \geq 48$ which is a better lower bound than 33.

We shall now study the case of lattices.

IV. LATTICES: QUADRATIC, TRIANGULAR, HYPERCUBIC

(1) QUADRATIC LATTICE (Q.L.)

We first examine the regular case $f = k$ cst. It is easy to check that any ball of radius R on Q.L. contains $2R^2 + 2R + 1$ vertices, therefore: $K = k(2R^2 + 2R + 1)$. Results on this case can be summarized in:

Theorem 4.1:

For any k and R , $C_R^{f=k}(\text{Q.L.}) = (2R^2 + 2R + 1)k = K$ and shifted colorings can be used. The minimal shift s is 2 if $R = 1$ and $s = 2R + 1$ otherwise.

Proof: By "shifted colorings" we mean that a first vertical line is selected and colored using K colors cyclically as in Proposition 3.1. Then for each successive vertical line we use the same pattern of colors but shifted by a constant vertical distance equal to s . Obviously such a coloring is essentially invariant under horizontal and vertical translations. Since $K \leq C_R^{f=k}(\text{Q.L.}) \leq k C_R^{f=1}(\text{Q.L.})$, it is enough to show our result for $k = 1$. If we represent the Q.L. using integer coordinates $(\mathbb{Z} \times \mathbb{Z})$ and if we number the colors by $\{0, 1, \dots, 2R^2 + 2R\}$ then a coloring with vertical shift s is defined by assigning one color to the origin. If we assign the color 0 to the origin then color c should be assigned to any vertex of coordinates:

$$(u, -us + v(2R^2 + 2R + 1) - c) \quad \begin{array}{l} u \text{ and } v \\ \text{in } \mathbb{Z} \end{array}$$

To satisfy the call coloring requirement we must have:

$2R \leq s$ and for symmetry reasons we can assume $s \leq R^2 + R$. Because of the invariance of the properties of such a coloring under translations, we need only to find what are

the possible values of s (if they exist) such that no conflict can occur for the color 0 when reused. The two closest vertices for the Manhattan metric to the origin where $c = 0$ correspond to:

$$u = \left\lfloor \frac{K}{s} \right\rfloor, v = 1 \quad \text{and}$$

$$u = \left\lfloor \frac{K}{s} \right\rfloor + 1, v = 1 \quad \text{with here } K = 2R^2 + 2R + 1.$$

No interference will occur if:

$$(1) \left\lfloor \frac{K}{s} \right\rfloor + K - \left\lfloor \frac{K}{s} \right\rfloor > 2R \quad \text{and}$$

$$(2) \left\lfloor \frac{K}{s} \right\rfloor + 1 - K + \left[\left\lfloor \frac{K}{s} \right\rfloor + 1 \right] s > 2R.$$

These conditions can easily be summarized by the relation:

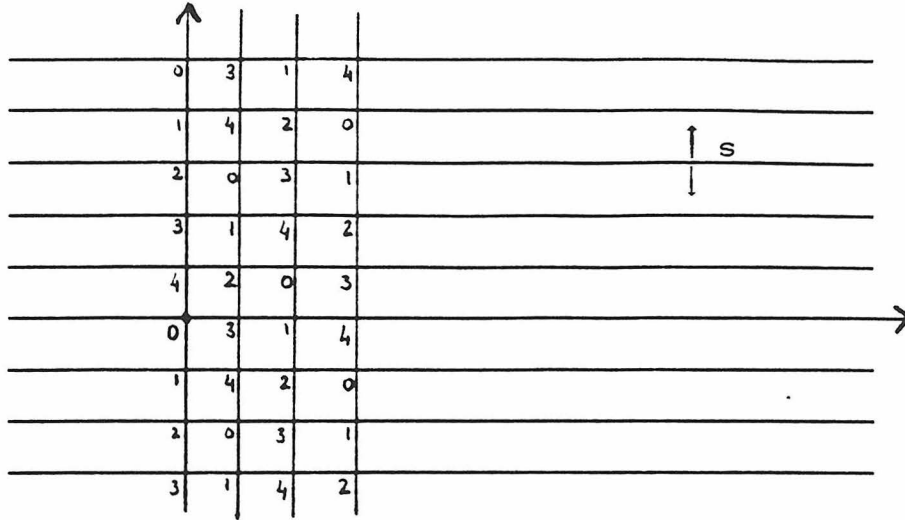
$$\left[\left\lfloor \frac{K}{s} \right\rfloor + 1 \right] (1+s) - 4R > 2R^2 + 1 > \left\lfloor \frac{K}{s} \right\rfloor (s-1).$$

For any value of R , this relation has several solutions. If we restrict ourselves to $2R \leq s \leq R^2 + R$ then the minimal solution occurs for $s = 2$ if $R = 1$ and $s = 2R + 1$ otherwise. Among other possible solutions we also have: $s = R^2 + 1$, $s = R^2 - d$ for any integer $d \geq v$ and as soon as $3d < \inf (R^2 - 4R + 2, R^2 - 2R - 1)$. For $R = 1, 2, 3, 4$ we have checked that these yield all the possible values for s with $2R \leq s \leq R^2 + R$.

$R = 1$	$s = 2$
$R = 2$	$s = 5$
$R = 3$	$s = 7, 10$
$R = 4$	$s = 9, 16, 17$

Using the symmetry if s satisfies (1) and (2) then also $(2R^2 + 2R + 2 - s)$ satisfies (1) and (2).

Example of coloring with $R = 1, s = 2$



Since N -gons can easily be embedded in Q.L. in the case of a general f a lower bound on $C_{R,K}^f(Q.L.)$ greater than K should be expected. Various arguments based on previous results lead to a linear upper bound in K . We have:

Theorem 4.2:

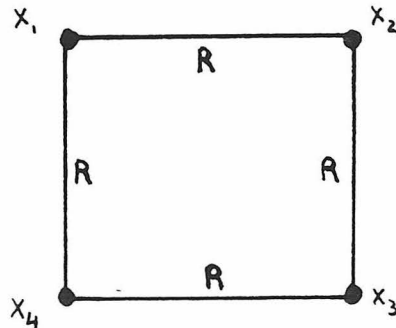
For any K :

if $R = 2m$: $K + \lfloor \frac{K}{4} \rfloor \leq C_{R,K}(Q.L.) \leq 2K$

if $R = 2m + 1$: $K + \lfloor \frac{K}{3} \rfloor \leq C_{R,K}(Q.L.) \leq 2K$.

Proof: Let us first consider the lower bounds.

If $R = 2m + 1$: consider the subgraph



Set $f = 0$ everywhere except at the corners x_i $i = 1, 2, 3, 4$.

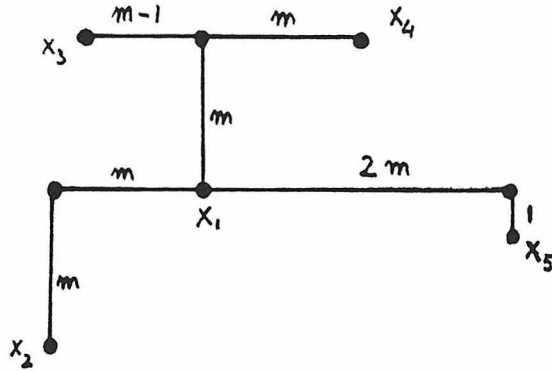
It is easy to check that any pair of corners interact, but because of the oddness of R , there is no ball of radius R containing all the x_i , $i = 1, 2, 3, 4$. If $K = 3n + d$ $d = 0, 1$, or 2 set:

$$f(x_1) = n + d$$

$$f(x_i) = n \quad \text{for } i = 2, 3, 4 .$$

Then f is in $\mathcal{F}_{R,K}$ and since all vertices interact: we need at least $3n + n + d = K + \lfloor \frac{K}{3} \rfloor$ colors.

If $R = 2m$: similar argument with a slightly more complicated subgraph.



Again, any two points interact but they are not all contained in a same ball of radius R . If $K = 4n + d$ $d = 0, 1, 2$ or 3 set:

$$f(x_1) = n + d$$

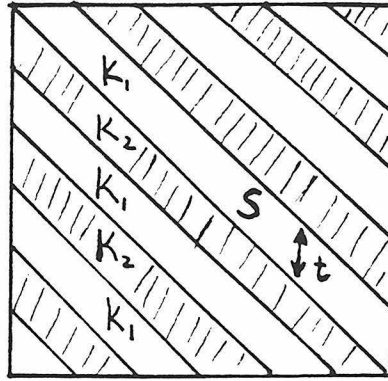
$$f(x_i) = n \quad i = 2, 3, 4, 5$$

$$f(x) = 0 \quad \text{everywhere else.}$$

Then f is in $\mathcal{F}_{R,K}$ and we need at least:

$$4n + n + d = K + \lfloor \frac{K}{4} \rfloor \text{ colors.}$$

To prove the upper bound $2K$ we are going to use the following coloring algorithm. We subdivide the lattice into contiguous identical strips. We use alternatively two sets of K colors, one for each strip. Experience shows that for the Q.L. diagonal strips (at a 45° angle) must be taken.

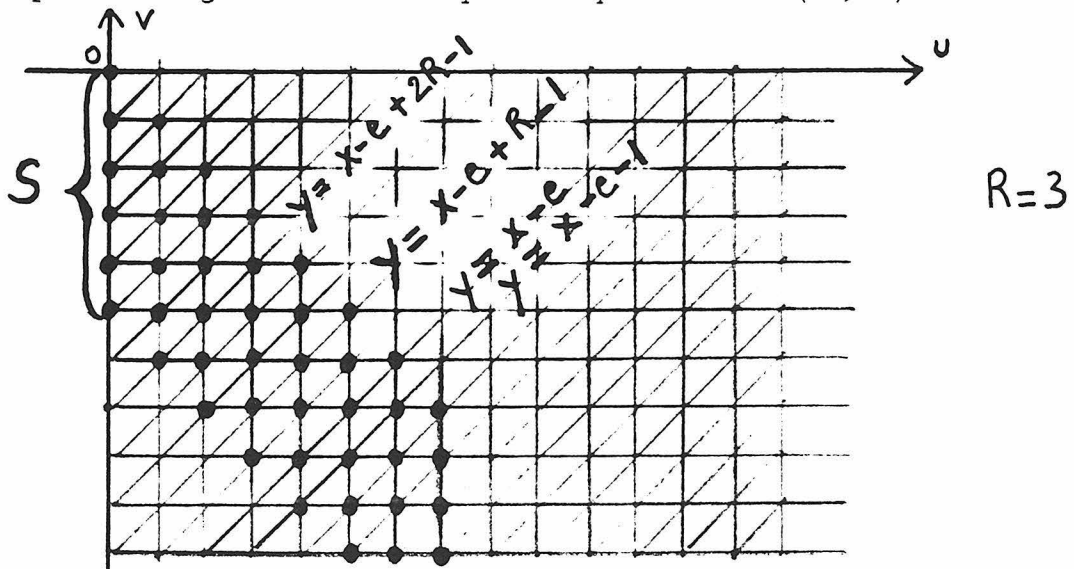


Let t be the constant thickness of a strip S measured by the number of lattice points belonging to S on a fixed vertical line. Then we need:

(a) t to be large enough so that no interference can occur between two points located on opposite sides of the strip.

(b) t to be small enough so that we can color S with only K colors.

Let t be equal to $2R$. It is easy to check (a), i.e., the distance between two points on each side of the strip is at least $2R + 1$. To prove (b), we assume that S is described in coordinates by the set of points (u, v) where u and v are in \mathbb{Z} and $-u - (2R-1) \leq v \leq -u$. In order to use the extension lemma, assume all points of S have been colored with K colors up to a diagonal line of equation $y = x - e$ ($e \geq 0$).



We want to extend the coloring to the points x of s located

on the line $v = u - e - 1$. Let $A = S_{\cap} \{v \geq u - e\}$.

Let $A(x) = S_{\cap} \{u - e \leq v \leq u - e - 1 + 2R\}$.

Let y_0 be any point in $S_{\cap} \{v = u - e - 1 + R\}$.

Then $d(y_0, x) = R$ and for any z in $A(x)$: $d(y_0, z) \leq R$.

The conditions for the extensions lemma are satisfied and therefore we can extend at once the call coloring to all the points x in $S_{\cap} \{v = u - e - 1\}$ using only K colors. Iterating this procedure yields a call coloring of S with K colors.

(2) TRIANGULAR LATTICE (T.L.)

As usual, we first examine the regular case. Any ball of radius R of T.L. contains $3R^2 + 3R + 1$ points. Therefore $K = (3R^2 + 3R + 1)k$. We are going to use the same shifted colorings.

Theorem 4.3:

For any k and R

$$C_R^{f=k}(\text{Q.L.}) = (3R^2 + 3R + 1)k = K$$

and shifted colorings can be used. If $R = 1$ the minimal possible shift is $s = 2$. For $R > 1$ a shift $s = 3R^2$ will always work.

Proof: Very similar to the Q.L. case. We can restrict ourselves to the case $k = 1$. Assume the coloring is given by:

$$(u, -us + v(3R^2 + 3R + 1) - c)$$

where u, v are integers and c belongs to $\{0, \dots, 3R^2 + 3R\}$. This time, since the symmetry is broken we can only assume:

$$2R \leq s \leq (3R^2 + 3R + 1) - (2R + 1) = 3R^2 + R$$

The properties of the coloring are still invariant under vertical and horizontal translations and therefore we can restrict ourselves to the color $c = 0$, the origin and the points with positive abscissa. The two closest vertices to the origin correspond to:

$$u = \left\lfloor \frac{K}{1+s} \right\rfloor \quad v = 1$$

$$u = \left\lfloor \frac{K}{1+s} \right\rfloor + 1 \quad v = 1$$

There will be no interference if their distance on the T.L. to the origin is greater than $2R$.

This yields:

$$(1) K - \left\lfloor \frac{K}{1+s} \right\rfloor s > 2R$$

$$(2) \left\lfloor \frac{K}{1+s} \right\rfloor + 1 > 2R \text{ if } K \geq \left[\left\lfloor \frac{K}{1+s} \right\rfloor + 1 \right] s \quad \text{or}$$

$$(2') \left[\left\lfloor \frac{K}{1+s} \right\rfloor + 1 \right] (s+1) - K > 2R \quad \text{otherwise.}$$

The combination (1) and (2) has a solution only in the case $R = 1$ which yields $s = 2$. With $R = 1$, (1) and (2') yield another possible shift $s = 4$. In general (1) and (2') reduce to:

$$\inf \left[\left\lfloor \frac{K}{1+s} \right\rfloor s + 1 - 2R, s \right] > K - \left\lfloor \frac{K}{1+s} \right\rfloor s > 2R$$

If $R > 1$ this reduces further to:

$$\left\lfloor \frac{K}{1+s} \right\rfloor + s + 1 - 2R > K - \left\lfloor \frac{K}{1+s} \right\rfloor s > 2R.$$

It is easy to see that $s = 3R^2$ always satisfies this relation for $R > 1$. It is by no means the unique solution. For instance $3R^2 - 1$ is also a solution as soon as $R \geq 4$ and $3R^2 + f$ ($0 \leq f \leq R$) is a solution as soon as $R \geq 3$. (For $R = 2$, $s = 14$ is also a possible shift).

The next theorem provides bounds for the general case.

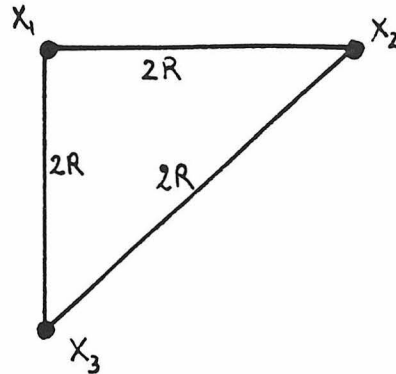
Theorem 4.4:

For any K :

$$K + \left\lfloor \frac{K}{2} \right\rfloor \leq C_{1,K} \text{ (T.L.)} \leq 2K$$

$$K + \left\lfloor \frac{K}{2} \right\rfloor \leq C_{R,K} \text{ (T.L.)} \leq 3K \quad (\text{for } R > 1).$$

Proof: For the lower bound consider the subgraph:



If $K = 2n + d$ $d = 0$ or 1 , let:

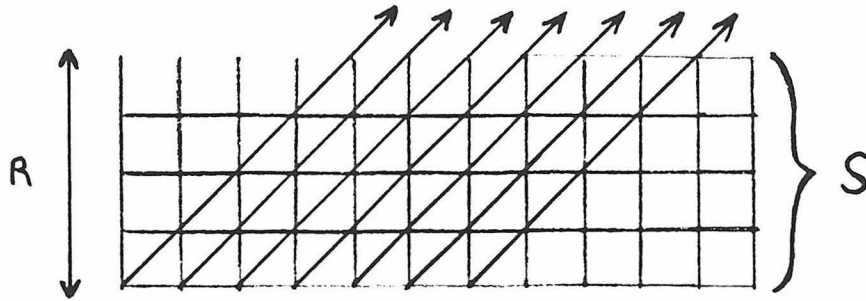
$$f(x_1) = n + d$$

$$f(x_2) = f(x_3) = n$$

$$f(x) = 0 \quad \text{elsewhere}$$

Then it is easy to check that f is in $\mathcal{F}_{R,K}$. Moreover $d(x_i, x_j) \leq 2R$ therefore the three points interact (and are not in a same ball of radius R). Therefore we need at least $2n + d + n$ colors.

In order to obtain the upperbound most related to cellular radio, we again use a decomposition into strips. Experimentation leads to the use of horizontal (or vertical) strips, assuming that the vertices of T.L. correspond to points with integer coordinates in a system of rectangular coordinates. If t is the thickness of the strip S , i.e. the number of lattice points of S on any vertical line, then as for Q.L. there is a tradeoff on the value of t . Examples can be constructed showing that if $t > R + 1$ then K colors are not sufficient to cover S . By iterative application of the extension lemma along successive diagonal lines (as in the figure)



one can show that if $t = R + 1$ then S is K colorable. The smallest distance between two points on each side of the strip is $R + 2$. Consequently if $R + 2 > 2R$ i.e. if $R = 1$ two sets of K colors in alternation on successive strips will suffice and $C_{1,K}(\text{T.L.}) \leq 2K$. On the other hand, if $R > 1$ the minimal distance between two points on each side of an adjacent pair of strips is $2R + 3$ which is sufficient. Therefore in general: $C_{R,K} \leq 3K$.

(3) N-HYPERCUBIC LATTICE: H_n

We consider H_n as represented by $\mathbb{Z} \times \dots \times \mathbb{Z} = \mathbb{Z}^n$. We have the:

Theorem 4.5:

For any $n \geq 2$, K , and R :

$$C_{R,K}(\text{Q.L.}) \leq C_{R,K}(H_n) \leq 2n K .$$

Proof: The lower bound is trivial since Q.L. is a subgraph of H_n for $n \geq 2$. For the upperbound we shall use Proposition 2.4. Let $B(0,2R) = \{(x_1, \dots, x_n) \in \mathbb{Z}^n : \sum |x_i| \leq 2R\}$. There are $2n$ balls of radius R centered at points of the form $(0, \dots, 0, \pm R, 0, \dots, 0)$. Let $x = (x_1, \dots, x_n)$ be a point in $B(0,2R)$ and assume without loss of generality that $x_k = |x_k| = \max_i |x_i|$ and let $x_k = R + y_k$. Then:

$$\sum |x_i| = \sum_{i \neq k} |x_i| + |R + y_k| \leq 2R .$$

$$\begin{aligned} \text{If } y_k \geq 0 \text{ then: } & \sum_{i \neq k} |x_i| + y_k \leq R . \\ \text{If } y_k < 0 \text{ then: } & \sum_{i \neq k} |z_i| - y_k \leq R . \end{aligned}$$

So x belongs to the ball centered at $(0, \dots, 0, R, 0, \dots, 0)$ (with an "R" in position k) with radius R . Therefore the $2n$ balls cover entirely $B(0, 2R)$. We can apply Proposition 2.4 and get the upperbound $2nK$. The upperbound can certainly be improved. For $n = 2$ we have already found $2K$ (instead of $4K$). Let us show, without attempting full generality, an example of improvement.

Theorem 4.6:

For any K and f in $\mathcal{F}_{1,K}(H_3)$ we have:

$$C_{1,K}(H_3) \leq 4K .$$

Proof: Let K_1, K_2, K_3, K_4 be four sets of K colors. The idea is to use K_1 and K_2 on alternating diagonal strips in the plane $z = 0$. Then, K_3 and K_4 similarly, in $z = 1$. Then K_1 and K_2 in $z = 2$, as for $z = 0$ but interchanging the role of K_1 and K_2 . More formally on points of the form $(n, 4m-n, z)$ or $(n, 4m-n+1, z)$ we use colors:

$$\begin{aligned} K_1 & \text{ if } z \equiv 0 \pmod{4} \\ K_3 & \text{ if } z \equiv 1 \pmod{4} \\ K_2 & \text{ if } z \equiv 2 \pmod{4} \\ K_4 & \text{ if } z \equiv 3 \pmod{4} \end{aligned}$$

For points of the form $(n, 4m-n+2z)$ or $(n, 4m-n+3, z)$ we use colors:

$$\begin{aligned} K_2 & \text{ if } z \equiv 0 \pmod{4} \\ K_4 & \text{ if } z \equiv 1 \pmod{4} \\ K_1 & \text{ if } z \equiv 2 \pmod{4} \\ K_1 & \text{ if } z \equiv 3 \pmod{4} \end{aligned}$$

K_3 if $z \equiv 3 \pmod{4}$

We leave as an exercise to check that this yields a call coloring.

V. GENERALIZATIONS

The call coloring problem on a graph $G = (V, E)$ can be extended as follows. Introduce a distance parameter d and require that calls at vertices x and y with $d(x, y) \leq d$ be assigned different colors. Denote by $C_d^f(G)$ the corresponding call chromatic number. In particular we have $C_R^f(G) = C_{d=2R}^f(G)$ and $C_{d=1}^{f=1}(G) = C(G)$. A subset X of V is a d -cluster if for any x and y in X then $d(x, y) \leq d$. We can then say that f is in $\mathcal{F}_{d,K}$ or K admissible with distance d if $\max_X \left(\sum_{x \in X} f(x) \right) \leq K$, the maximum being taken over all possible d -clusters. Define $C_{d,K}(G)$ as usual. It should be noticed that d clusters do not always correspond to balls, even when d is even. We leave as an exercise to show that all the previous results can be extended. In particular we have:

$$(1) C_{d,K}(T) = K \quad \text{for any tree } T$$

$$(2) \text{ For any } N\text{-gone } (G_N) \text{ with } N = b(d+1) + a \quad 0 \leq a \leq d$$

$$C_d^{f=k}(G_N) = \begin{cases} ka & \text{if } b=0 \\ (d+1)k + \left\lceil \frac{ka}{b} \right\rceil & \text{otherwise} \end{cases}$$

Moreover, for N large enough:

$$C_{d,K}(G_N) = K \text{ or } K + 1$$

$$(3) C_{d,K}(Q.L.) \leq 2K$$

$$(4) C_{d,K}(T.L.) \leq 2K \quad \text{for } d = 1, d = 2$$

$$C_{d,K}(T.L.) \leq 3K \quad \text{for } d > 2$$

A striking feature of the previous analysis is that at least in the case $R = 1$ or $d \leq 2$ we always have: $C_{d,K} \leq 2K$ and $C_{R,K} \leq 2K$ for trees, N -gones and planar lattices. It is therefore natural to conjecture whether this could be a characteristic property of all planar graphs. In fact even more generality can be attempted if we try to extend the Heawood theorem as follows. Let S_g denote an (orientable)

surface of genus g . Then the chromatic number $C(S_g)$ is the maximal chromatic number among all the graphs G that can be embedded in S_g . Heawood theorem states that:

$$C(S_g) = \left\lfloor \frac{7 + \sqrt{1 + 48g}}{2} \right\rfloor$$

The planar case $g = 0$ is of particular interest and will be referred to as 4CT (four color theorem). In a similar fashion we can define the quantities $C_{d,K}(S_g)$ and $C_{R,K}(S_g)$ and the problem is to study these functions of three variables g, K and d (or R). In particular, say for fixed g and R , is it possible to find an upperbound which is polynomial in K , or even linear as in the previous examples? We shall describe some partial results in these directions.

If $G = (V, E)$ let G^n be the graph (V, E^n) where $(x, y) \in E^n$ iff $d(x, y) \leq n$ in G . We then trivially have:

$$C_{d,K}(G) \leq C_d^{f=1} K \leq C(G^d)K \text{ and } C_{R,K}(G) \leq C(G^{2R})K .$$

Let $c(g) = \left\lfloor \frac{7 + \sqrt{1 + 48g}}{2} \right\rfloor$. The next theorem describes a lower bound on $C_{K,R}(S_g)$ and a precise relation to the Heawood theorem.

Theorem 5.1:

(1) For any K, R and g :

$$C_{R,K}(S_g) \geq c(g) \left\lfloor \frac{K}{2} \right\rfloor + i \text{ where } i = 0 \text{ or } 1 \text{ and } K \equiv i \pmod{2}$$

(2) $C(S_g) = c(g)$ (Heawood theorem) is equivalent to the statement:

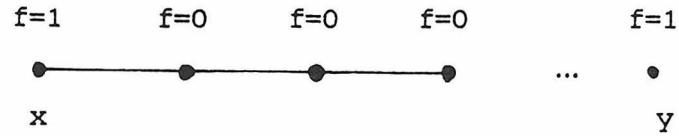
$$C_{R,K=2}(S_g) = c(g)$$

Proof: (1) Consider the following construction. Take the graph $K_n (n > 2)$. Let F_n be the graph obtained by inserting $2R - 1$

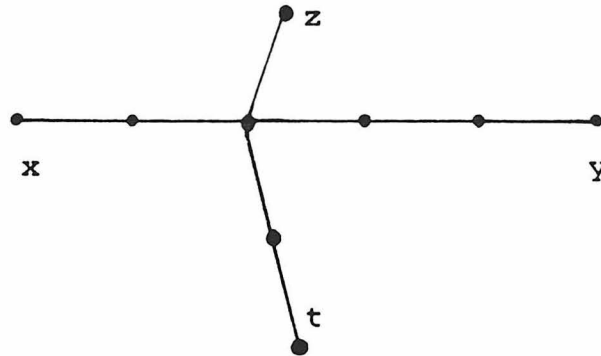
vertices along each edge of K_n . Define a function $f: V(F) \rightarrow N$ by $f(x) = 0$ if $d(x) = 2$ and $f(x) = \lfloor \frac{K}{2} \rfloor$ if $d(x) > 2$. (In the case where K is odd we set $f(x) = \lfloor \frac{K}{2} \rfloor$ on all vertices with $d(x) > 2$ except for one of them, say y , for which $f(y) = \lfloor \frac{K}{2} \rfloor + 1$). A trivial check shows that f is in $\mathcal{F}_{R,K}$. In addition: $C_{R,K}^f(F_n) = n \lfloor \frac{K}{2} \rfloor + i$ where $i = 0$ or 1 and $K \equiv i \pmod{2}$. Notice for later that $C(F_n) = 2$ if R is odd, 3 otherwise and that F_n is homeomorphic to K_n . Therefore if $n \leq c(g)$, F_n can be drawn on S_g , proving our first assertion.

(2) Assume first that: $C_{R,K=2}^f(S_g) = c(g)$. Let G be any graph embeddable in S_g . Then we have seen (Proposition 2.1) that we can construct a graph $S_R(G)$ and a call function f in $\mathcal{F}_{R,2}$ such that: $C(G) = C_R^f(S_R(G))$. The construction shows that $S_R(G)$ and G have exactly the same genus. Therefore: $C(G) \leq c(g)$. On the other hand the bound is attained by taking G equal to a complete graph.

For the converse we assume the Heawood theorem. Let g be embeddable in S_g and let f be in $\mathcal{F}_{R,2}$. We know (Proposition 2.2) that we can construct a graph $\psi_R^f(G)$ such that: $C_R^f(G) = C(\psi_R^f(G))$. We need to verify that in this case the genus of G is not increased by the operation $\psi_R^f(G)$. If for some vertex $f(x) = 2$, then for any y such that $d(x,y) \leq 2R$ we have $f(y) = 0$. It is easy to see that ψ_R^f will transform x into a complete graph on 2 points completely disconnected from the rest, and this cannot increase the genus of G . Consider now vertices x , for which $f(x) = 1$. ψ_R^f creates a new edge only between two points x and y such that: $f(x) = f(y) = 1$ and $1 < d(x,y) \leq 2R$. Then we necessarily have the picture:



We can assume that the new edge from x to y in $\psi_R^f(G)$ goes along the shortest path joining x to y in G . Suppose now for contradiction that two such newly created edges cross. Then, in G , we would have the situation:



with $f(x) = f(y) = f(z) = f(t) = 1$ and $f = 0$ for the vertices on the path x to y and z to t . Also $d(x,y) \leq 2R$ and $d(z,t) \leq 2R$. But then there would exist a point v on the paths such that $f \in \mathcal{F}_{R,2}(G)$ is violated by the ball $B(v,R)$. So ψ_R^f does not increase the genus of G . Therefore $C_{R,K=2}^f(G) \leq c(g)$ and again equality can be achieved by using complete graphs.

Let us consider the case of planar graphs more carefully. We just saw that $C_{R,2}(S_0) = 4$. We are going to prove:

Theorem 5.2

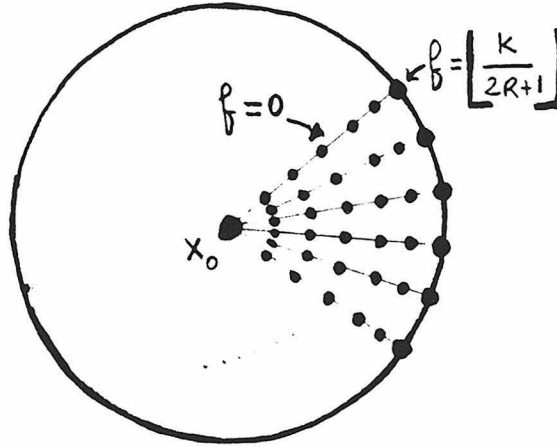
(1) For any radius $R \geq 1$ and any $K \geq 2R + 1$:

$$K + 4R \left\lfloor \frac{K}{2R+1} \right\rfloor \leq C_{R,K}(S_0)$$

(2) For any K :

$$C_{1,K}(S_0) \leq 5K .$$

Proof (1) This of course shows that $2K$ colors are not enough for certain planar graphs even with radius $R = 1$. The lower bound is attained by the following special wheel graph. Start with an N -gone with $N = 4R + 1$ and $f(x) = \lfloor \frac{K}{2R+1} \rfloor$ everywhere (in particular $f(x) \neq 0$) . By our previous result on N -gons $(4R+1) \lfloor \frac{K}{2R+1} \rfloor$ colors are already necessary to cover the N -gone. Now add a new vertex x_0 with $f(x_0) = K - \lfloor \frac{K}{2R+1} \rfloor$. Finally connect x_0 to all the previous $4R + 1$ vertices of the N -gone via $4R + 1$ edges. Along each one of these $4R + 1$ edges insert $2R - 1$ additional vertices for which f is equal to zero.



The graph obtained is planar, f is in $\mathcal{F}_{R,K}$ and any two points interact. Therefore:

$$C_{R,K}(S_0) \geq K - \lfloor \frac{K}{2R+1} \rfloor + (4R+1) \lfloor \frac{K}{2R+1} \rfloor \quad \text{or}$$

$$C_{R,K}(S_0) \geq K + 4R \lfloor \frac{K}{2R+1} \rfloor$$

(2) Assume for contradiction that $G = (V,E)$ is the smallest

planar graph with a given call function f in $\mathcal{F}_{1,K}(G)$ which is not $5K$ call colorable. Classically, using Euler's formula, it is easy to see that G must have at least one vertex x_0 of degree at most 5. By assumption if H is the graph obtained from G by removing x_0 , then H is $5K$ call colorable for the restriction of f to $V - \{x_0\}$. The restriction of f is trivially in $\mathcal{F}_{1,K}(H)$. We then have:

$$\sum_{B(x_0, 2)} f(x) \leq 5K - 4f(x_0).$$

Therefore if we have $5K$ colors, we can consistently extend the call coloring of H to x_0 and hence to G .

As a conclusion, we see that in the planar case with radius $R = 1$ and $K \geq 3$ the following inequality holds:

$$K + 4 \left\lfloor \frac{K}{3} \right\rfloor \leq C_{1,K}(S_0) \leq 5K$$

Additional results have been obtained in this area for instance by looking at small values of K , arboricity or special classes of graphs (regular, outerplanar, ...) . The situation being still unclear we reserve them for a later publication. We end up with an example.

Proposition 5.3:

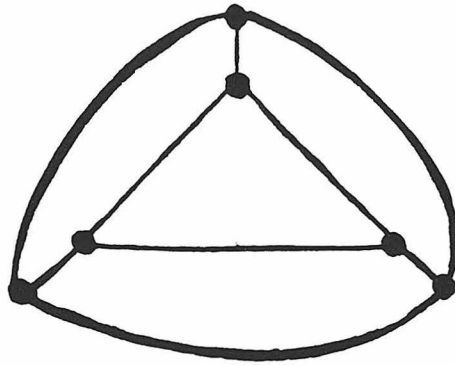
For planar cubic graph (P.C.) :

$$6 \leq C_{R=1}^{f=1}(\text{P.C.}) \leq 9$$

If all the faces have length even or equal to three, then:

$$6 \leq C_{R=1}^{f=1}(\text{P.C.}) \leq 8$$

Proof: Notice that here $K = 4$. For the lower bound, just consider the graph:



An upperbound of 10 is immediate by considering the degrees (or using Proposition 2.4) . By the Brook theorem we also know the case of equality: if G is planar cubic then G^2 must be a complete graph on 10 points. By a result of Hoffman and Singleton [IBM Journal Nov. 1960] on Moore graphs, this can occur iff G is the Petersen graph which is non planar. Therefore, $C_{R=1}^{f=1}(\text{P.C.}) \leq 9$. In the construction of G^2 , new edges are added within each non triangular face. If a face has even length $2n$ the corresponding additional edges can be partitioned into two n -gons. The face and one of the n -gons is still planar. Therefore G^2 can be decomposed into two planar graphs and so is 8 colorable using 4CT if every face is triangular or of even length.

VI. CONCLUSION: OPEN QUESTIONS

We have shown several results where the classical notion of chromatic number has been extended in two directions: by assigning several colors to each vertex via the function f and by the introduction of the radius R . Sharper bounds, other classes of graphs and possible connections to the Heawood and the 4CT, both in the orientable and non orientable case, require additional exploration. Other notions of Graph Theory and Extremal Graph Theory could be reexamined along the same lines.

In view of applications, the problem treated seems to be slightly more general than cellular radio. It is possible to imagine other situations where resources or computations need to be distributed over a network with some "interference" condition. As far as cellular radio is concerned, our upperbounds are probably still too large for current technology. One question to be investigated seems to be whether, by disregarding a small fraction of the calls, the upperbound can be lowered significantly to a value close to K . If so, what are the corresponding good coloring algorithms?

SOME CONTRIBUTIONS TO THE THEORY OF NEURAL NETWORKS

Abstract: We investigate some generalizations of neural networks using acyclic orientations and algebraic threshold functions. We estimate the number of acyclic orientations of the hypercube corresponding to energy functions of degree d and analyze stable states especially in terms of invariances under the action of a group of isometries. Combinatorial complexity results on the optimization of algebraic forms over the hypercube and a reduction algorithm are introduced.

I. INTRODUCTION

In 1982, J. J. Hopfield, in an attempt to understand the emergence of collective computational abilities in physical systems and networks of neurons, presented a model that has been since the source of a great deal of work. The original simple idea and several of its derivations have already been applied to a variety of contexts ranging, among others, from content addressable memories and circuits architectures to learning algorithms and combinatorial optimization. We refer the interested reader to the short bibliography at the end.

In the original Hopfield discrete model, a neural network consists of n pairwise interconnected devices or neurons, each one being in one of two possible states, $+1$ or -1 . The state of the system is therefore represented by a vector $X = (x_1, \dots, x_n)$ belonging to the hypercube H^n .

The synaptic connections are described by a real symmetric matrix $a = (a_{ij})$ with the additional property: $a_{ii} = 0$ for any i . Moreover, to each neuron i is associated a real threshold t_i . Randomly and asynchronously each neuron changes its state according to the following rule. If x_i^+ and x_i^- are respectively the state of neuron i before and after the corresponding updating step then:

$$x_i^+ = \text{sgn} \left[\sum_{j=1}^n a_{ij} x_j - t_i \right]$$

$$\text{If } \sum_{j=1}^n a_{ij} x_j - t_i = 0 \text{ then } x_i^+ = x_i^-$$

This system possesses a fundamental emergent property namely that no matter what the starting state is and no matter in which fashion the neurons "decide" to update themselves it will always converge to a stable state. The reason behind this key fact is the existence for the network of an energy function which is decreasing when the previous algorithm is applied. If we consider the quadratic form:

$$E(x) = - \sum_{i < j} a_{ij} x_i x_j + \sum_{i=1}^n t_i x_i$$

$$E^+ - E^- = - \left[x_i^+ - x_i^- \right] \left[\sum_{j=1}^n a_{ij} x_j - t_i \right]$$

Therefore $E^+ - E^- \leq 0$ and since there are only 2^n possible states the system must reach a stable state. There exists a wealth of interesting questions concerning the properties of this model and of its possible uses.

II. FIRST GENERALIZATION: ACYCLIC ORIENTATIONS

The algorithm above consists of a sequence of nonlinear operations describing the evolution of the neural network from the point of view of the neurons, or of the circuit which simulates them. Yet, a different but totally equivalent description can be given in the space of states, i.e. on the hypercube H^n of n -tuples of $(1,-1)$ coordinates.

Starting from one state X with energy $E(X)$:

- (1) choose a new neighbor Y
- (2) compute $E(Y)$
- (3) if $E(Y) < E(X)$ move to Y
if not go to step (1).

It is essential to notice for our point that the discrete dynamical behavior does not depend at all on the actual value of the energies but only on the partial ordering they induce on the vertices of the hypercube. Moreover different rules can be applied for the choice of Y . For instance we can select the neighbor Y with lowest energy (Optimal Adjacency Algorithm) or choose among all the better neighbors with equal probability (Better Adjacency Algorithm). Also in the case where: $E(X) = E(Y)$ additional rules could be adopted. For instance, a fixed orientation $X \rightarrow Y$ or $Y \rightarrow X$ can be chosen a priori. The description of the original Hopfield model is equivalent in this case to the removal of the edge (X,Y) .

We can introduce the following generalization:

Let $G(V,E)$ be a graph with the metric induced by the length of the shortest path between points and R be a radius.

Let us assume that a partial ordering has been defined on the vertices V of G which is compatible with R , i.e. such that:

$$\text{if } d(X,Y) \leq R \text{ then } X < Y \text{ or } Y < X.$$

Define then the local algorithm:

Starting from a state X

- (1) choose a new vertex Y such that $d(X,Y) \leq R$
- (2) if $Y < X$ move to Y otherwise go to step (1).

In optimization problems, it might be useful to progressively reduce the value of R . This point needs to be investigated and from now on we shall assume as usually that $R = 1$.

If $R = 1$, it only means that we have directed the edges of G . There are of course $2^{|E|}$ possible orientations. In the general case this local algorithm is not guaranteed to converge. But it is easy to show that on any finite graph G the local algorithm will converge iff we have an acyclic orientation (A.O.) i.e. iff the orientation of the edges in E is not constant along any cycle of G . This is the case of the hypercube H^n under the energy function E . There is therefore a one to one correspondence between acyclic orientations of G and dynamical behaviors on G induced by the local algorithm (of course for a fixed probability distribution for the choice of the neighbors).

Any injective function $f:V \rightarrow O$ where O is a totally ordered set will automatically induce a linear ordering of the vertices V and also an A.O. of the edges of G by the relation:

$$X \rightarrow Y \text{ iff } Y < X \text{ iff } f(Y) < f(X) \left[\begin{array}{l} \text{with respect to} \\ \text{the ordering of } O \end{array} \right]$$

Since every partial order can be extended to a linear order, the converse is also true: for any acyclic orientation we can find a function: $f:V \rightarrow \{1,2,\dots,|V|\}$, i.e. a total ordering of the vertices via the usual order on the integers, such that the original A.O. is identical to the one induced by f . Later it will be useful to think of the integers $\{1,2,\dots,|V|\}$ as being "thrown" randomly on G . There exists therefore a basic many to one map from the set $L(G)$ of linear orderings on the vertices of G into $A(G)$, the set of A.O. of G or dynamical behaviors on G . We shall define the capacity $C(G)$ of G in bits to be the logarithm base 2 of $|A(G)|$.

In the case of the Hopfield model, $G = H^n$ and the function f is the quadratic form corresponding to the energy E . Two discrete neural networks with different energy function but with the same A.O. on the hypercube H^n are statistically indistinguishable on the basis of their behavior.

Notice that $|L(G)| = |V|!$ and theoretically there exists a way of counting $|A(G)|$. If $P_G(\lambda)$ is the chromatic polynomial of G (i.e. $P_G(\lambda)$ is the number of different colorings of G using λ colors) then by a theorem of Stanley [Stanley,1973] we have: $|A(G)| = |P_G(-1)| =$ the sum of the absolute value of the coefficients of $P_G(\lambda)$.

Notice also that there exists a subset of $A(G)$ for which local and global minima coincide. (i.e. with a unique local-global minima). Let $G(G)$ be this subset.

From now on we shall confine ourselves to the case of the hypercube H^n . In a later section we shall treat the problem of enumerating all the acyclic orientations on the hypercube and compare it to those induced by quadratic

energies. The more fundamental question we would like to understand is whether there exists differences between random landscapes on the hypercube and landscapes created by quadratic energies. If so, can we take advantage of these differences for example in optimization problems.

III. SECOND GENERALIZATION: ALGEBRAIC THRESHOLD FUNCTIONS

The original Hopfield model is based on a quadratic energy function, yet we have seen that almost any function $f: H^n \rightarrow O$ where O is a totally ordered set defines uniquely a dynamical behavior. We are going to introduce and study a class of functions f which leads to non quadratic energies. For this we need some additional notation.

Let $N = \{1, 2, \dots, n\}$. Let x_i ($i=1, 2, \dots, n$) denote the coordinates of a vertex X of the hypercube ($x_i = \pm 1$).

If $I \subset N$ let $x^I = \prod_{i \in I} x_i$ (notice that on H^n $x_i^{2m} = 1$, therefore only 0 and 1 powers of the variables need to be considered).

If $I \subset P(N)$ then an algebraic form in n variables based on I with coefficients in A is a polynomial expression of the type:

$$P_n(X) = \sum_{I \in I} \alpha_I x^I \text{ and } \alpha_I \in A .$$

An algebraic form in n variables $P_n^d(X)$ is said to be of degree d if it is the form:

$$P_n^d(X) = \sum_{|I| \leq d} \alpha_I x^I .$$

It is said to be homogeneous of degree d if it is of the form:

$$\bar{P}_n^d(X) = \sum_{|I|=d} \alpha_I x^I .$$

Let $F_n^I(A)$, $F_n^d(A)$, $\bar{F}_n^d(A)$ be the set of all algebraic forms in n variables, with coefficients in A respectively: based on I , of degree d , homogeneous of degree d . Interesting possibilities for A are: $A = \mathbb{C}$, $A = \mathbb{R}$, $A = \mathbb{Q}$, $A = \mathbb{Z}$, $A = \{-1, 0, 1\}$, $A = \text{GF}(q) \dots$. These forms can be defined on any graph where a "system of coordinates" for the vertices has been defined.

A homogeneous form of degree d on H^n depends on $\binom{n}{d}$ coefficients. A general form of degree d depends on:

$$r(n,d) = \sum_0^d \binom{n}{k} \text{ coefficients.}$$

If A is a field, $F_n^d(A)$ can be trivially seen as the vector space $A^{\binom{n+d-1}{d}}$. Notice also that for forms \bar{P}_n^d in \bar{F}_n^d we have:

$$\bar{P}_n^d(-X) = (-1)^d \bar{P}_n^d(X)$$

and this symmetry is reflected in the dynamical behavior \bar{P}_n^d induces on H^n .

A switching function $f(x_1, \dots, x_n)$ of n binary variables is a function $f: H^n \rightarrow \{0,1\}$. f is separable by a form of degree d if we can find $P_n^d \in F_n^d(A)$ such that the algebraic curve $P_n^d = 0$ in \mathbb{R}^n separates the "on" set $f^{-1}(1)$ from the "off" set $f^{-1}(0)$. In other words:

$$f(X) = 0 \Leftrightarrow P_n^d(X) < 0$$

$$f(X) = 1 \Leftrightarrow P_n^d(X) > 0.$$

A switching function which is separable by a form of degree d is called an algebraic threshold function of degree d . Let $T_n^d(A)$ (resp. $\bar{T}_n^d(A)$) denote the set of all algebraic (resp. homogeneous) threshold functions of degree d in n variables with coefficients in A .

So far, in practice, quadratic form energies are the most widely used. In a context of optimization problems we shall see that the complexity covered by $F_n^2(A)$ is already staggering enough for our current possibilities and in some

sense energies functions in $F_n^d(A)$ can be reduced to forms in $F_m^2(A)$ but at a high cost ($m \gg n$).

Yet, for instance, the problem of the capacity (as defined in [Abu Mostafa,1985]) of neural networks with higher-degree energy functions is of interest and not of a purely academic nature. Indeed hard wired circuits simulating such energy functions could be implemented. (For instance using a combination of fast and slow operational amplifiers [Baum,1985]). Moreover, there exists a wide class of problems with constraints that cannot be converted into the optimization of a quadratic form in a simple fashion. Several problems of combinatorial designs and coding theory amount to the construction of a binary $m \times l$ matrix $M = (m_{ij})$ with $m_{ij} = \pm 1$ and some additional restrictions on the rows and columns. Typical constraints are of the form: "the Hamming distance between row a and row b is c_{ab} ".

This can be expressed as:

$$(1) \quad \sum_{k=1}^l m_{ak} m_{bk} = 1 - 2c_{ab}.$$

This kind of equation cannot be converted directly into the optimization of a quadratic form. Yet this is easy with a form in F^4 in the variables m_{ij} :

$$P^4 = \sum_{\substack{a,b \\ a < b}} \left[\sum_{k=1}^l m_{ak} m_{bk} - 1 + 2c_{ab} \right]^2$$

Trivially $P^4 \geq 0$ and the minimum 0 of P^4 occurs iff (1) holds for every a and b .

It is not completely impossible that progress in these

directions might shed some light on combinatorial problems, the most famous one being the existence of a projective plane of order 10. (i.e. a certain 111×111 matrix). Incidentally, according to [Wilson,Hall,1986] the smallest interesting binary matrix the existence of which is unknown has dimension 22×33 . Neural networks of this size have already been designed though based on quadratic energy functions. These circuits are known to converge towards states of low energy though they are not guaranteed to reach the optimum. Yet the speed of convergence of hard wired networks is very high and a large number of trials with various starting states becomes possible. Information contained in partially optimal solutions might be useful in restricting the size of a systematic computer search for the optimum.

Let us assume that a given neural network and the corresponding A.O. of H^n is defined by an energy function P_n^d in $F_n^d(A)$. If we look at what happens when we are updating "neuron i" we can write:

$$P_n^d(X) = x_i P_{n-1}^{d-1} + Q_{n-1}^d$$

where P_{n-1}^{d-1} is a form of degree $d-1$ in the variables $(x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_n)$ and Q_{n-1}^d is a form of degree d in the same variables. The energy difference between the two states: $(x_1, \dots, x_{i-1}, 1, x_{i+1}, \dots, x_n)$ and $(x_1, \dots, x_{i-1}, -1, x_{i+1}, \dots, x_n)$ depends only on the form P_{n-1}^{d-1} . In other words each neuron needs only to compute locally the sign of an algebraic form of degree $d-1$ in $n-1$ variables. Moreover, each neuron simulates an algebraic threshold function in T_{n-1}^{d-1} . The quadratic case is of course particularly nice since only linear forms in $n-1$ variables are computed. Whereas in the case $d=2$ the connection between neurons form a simple graph, for $d > 2$ we have a hypergraph (i.e. edges are clusters of neurons rather than simple pairs).

IV. PRELIMINARIES AND EXAMPLE

As we have seen, we want to study some properties related to the three maps:

$$\psi_1: L(H^n) \rightarrow A(H^n)$$

$$\psi_2: F_n(\mathbb{R}) \rightarrow A(H^n)$$

$$\psi_3: F_n(\mathbb{R}) \rightarrow L(H^n)$$

ψ_2 and ψ_3 are not defined everywhere on $F_n(\mathbb{R})$ since a form P can take the same value on two vertices X and Y . If $P(X) = P(Y)$ we cannot order the vertices of H^n linearly. In addition, if (X, Y) is an edge of H^n there is a difficulty in the definition of the corresponding A.O. The domain of ψ_3 is a proper subset of the domain of ψ_2 which is a proper subset of $F_n(\mathbb{R})$. In a later section on NP completeness we will require also that $P \in F_n(\mathbb{Z})$. These are all technical difficulties that can be easily overcome as shown in the following proposition.

Proposition 4.1:

(1) Let $P \in F_n^d(\mathbb{R})$. Then we can construct an algebraic form $Q \in F_n^d(\mathbb{R})$ such that $Q(X) \neq Q(Y)$ for any two vertices X and Y . Also if $P(X) < P(Y)$ then $Q(X) < Q(Y)$.

(2) Let $Q \in F_n^d(\mathbb{R})$ such that $Q(X) \neq Q(Y)$ for any two vertices X and Y . Then we can construct $R \in F_n^d(\mathbb{Q})$ such that:

$$Q(X) < Q(Y) \text{ iff } R(X) < R(Y) .$$

(3) Let $R \in F_n^d(\mathbb{Q})$ such that $R(X) \neq R(Y)$ for any two vertices X and Y . Then we can construct $S \in F_n^d(\mathbb{Z})$ such that $R(X) < R(Y)$ iff $S(X) < S(Y)$.

Proof: (1) Assume $X = (x_1, \dots, x_n)$ $Y = (y_1, \dots, y_n)$ are two vertices such that $P(X) = P(Y)$. Let $c = \min |P(Z) - P(T)|$ the minimum being taken over all vertices Z, T such that: $P(Z) \neq P(T)$. Then if $P(X) = \sum_{|I| \leq d} a_I x^I$ we can construct a new form

$$\tilde{Q}(X) = \sum_I (a_i + h_I) x^I \text{ with: } |h_I| < \frac{c}{2r(n, d)} \text{ and } \sum_I h_I x^I \neq$$

$\sum_I h_I y^I$ (for instance if X and Y differ in position i let $h_{\{i\}} =$

$\frac{c}{3r(n, d)}$ and $h_I = 0$ for $I \neq \{i\}$).

Then obviously $\tilde{Q}(X) - \tilde{Q}(Y) = \sum_I h_I x^I - \sum_I h_I y^I \neq 0$. In addition if T and Z are two vertices such that: $P(T) < P(Z)$ then:

$\tilde{Q}(Z) - \tilde{Q}(T) = P(Z) - P(T) + \sum_I h_I z^I - \sum_I h_I t^I$. Now $P(Z) - P(T) \geq c$ by assumption and:

$$|\sum_I h_I z^I - \sum_I h_I t^I| \leq 2 \sum_I |h_I| < c.$$

Therefore $\tilde{Q}(Z) - \tilde{Q}(T) > 0$ and \tilde{Q} preserves the partial ordering induced by P . Iterating this procedure a finite number of times yields the desired form Q .

(2) Essentially the same procedure. If $Q(X) = \sum_{|I| \leq d} a_I x^I$. Let h_I be such that: $a_I + h_I$ is a rational and $|h_I| < \frac{c}{2r(n, d)}$. Then $R(X) = \sum_I (a_I + h_I) x^I$ belongs to $F_n^d(\mathbb{Q})$ and preserves the ordering induced by Q .

(3) This is trivial since for any $P \in F_n^d(\mathbb{R})$ the form $\lambda P + \mu$ ($\lambda > 0$) induces exactly the same A.O. and total ordering as P . Therefore one need only multiply the given rational form by the absolute value of the common denominator of all the coefficients.

In real circuits the parameters a_I are only known as rationals. Because of the theorem above, it does not really matter for this point whether the coefficients are in \mathbb{R} , \mathbb{Q} , or \mathbb{Z} . From now on we shall only consider the restriction of ψ_2 and ψ_3 to their domains. We shall write: A_n^d (resp. \bar{A}_n^d) for $\psi_2(F_n^d(\mathbb{R}))$ (resp. $\psi_2 \bar{F}_n^d(\mathbb{R}))$ i.e. for the A.O. generated by forms of degree d and similarly: L_n^d (resp. \bar{L}_n^d) for $\psi_3(F_n^d(\mathbb{R}))$ (resp. $\psi_3 \bar{F}_n^d(\mathbb{R}))$ i.e. for the linear ordering of the vertices of H^n generated by forms of degree d . For d even, \bar{L}_n^d is undefined.

It should be noticed that the two equivalence relations on $F(\mathbb{R})$:

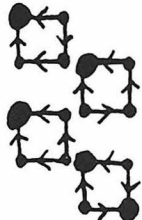
$$P \sim Q \text{ iff } \psi_2(P) = \psi_2(Q) \quad \text{and}$$



$$P \sim Q \text{ iff } \psi_3(P) = \psi_3(Q)$$

are not compatible with the vector space operations defined on $F(\mathbb{R})$.

Our purpose will be to obtain some information about the increasing sequences A_n^d (and L_n^d) when d varies from one to n .

Example: $n = 2$

Quantity:	Type of A.O.	Number of linear orderings:
4 ×		1 × 4 = 4
4 ×		1 × 4 = 4
4 ×		2 × 4 = 8
2 ×		4 × 2 = 8
<u>Total:</u> 14		24 = 4!

We have $|L(H^2)| = 4! = 24$ $|A(H^2)| = 14$. There are only two cyclic orderings. It is easy to see that only the type:  can be described with a linear form and only the type:  can be

described by a homogeneous quadratic form. On the other hand all possible A.O. can be described using a quadratic form.

Therefore:

$$\begin{aligned} A_2^2 &= 14 & \bar{A}_2^2 &= 2 & A_2^1 &= 4 = \bar{A}_2^1 \\ L_2^2 &= 24 & \bar{L}_2^2 &= \text{undefined} & L_2^1 &= 8 = \bar{L}_2^1 \end{aligned}$$

However, this situation is not typical and even for $n = 3$ the computation is difficult. To compute bounds on $|A_n^d|$ we extend the technique found in [Abu-Mostafa and St. Jacques,1985].

V. BOUNDS AND CAPACITY

Proposition 5.1:

For every $I \subset P(N)$ and for $n \geq d \geq 1$ we have:

$$(1) |T_n^I(\mathbb{R})| \leq |T_{|I|-1}^1(\mathbb{R})|$$

$$(2) |\bar{T}_n^d(\mathbb{R})| \leq |T_{\binom{n}{d}-1}^1(\mathbb{R})| \text{ and}$$

$$(3) |T_n^d(\mathbb{R})| \leq |T_{r(n,d)-1}^1(\mathbb{R})|$$

Proof: We shall use the same notation for the threshold function and the associated algebraic form. If $Q \in T_n^I(\mathbb{R})$ then Q can be seen as an element of $\mathbb{R}^{|I|}$. This element in $\mathbb{R}^{|I|}$ defines an algebraic linear form P in $|I| - 1$ variables. If P takes the value 0 for some vertex of $H^{|I|-1}$ we can slightly perturb P as in Proposition 4.1, so that P can be seen as an element of $T_{|I|-1}^1(\mathbb{R})$. Therefore we can define a map $f: T_n^I(\mathbb{R}) \rightarrow T_{|I|-1}^1(\mathbb{R})$.

Let us show that f is injective. If S, T are in $T_n^I(\mathbb{R})$, $S \neq T$, then there exists a vertex $X = (x_1, \dots, x_n)$ of H^n such that $S(X) > 0$ and $T(X) < 0$. Let Y be the vector on $H^{|I|-1}$ which components are $(x^I)_{I \in I}$. Then necessarily: $f(S)(Y) > 0$ and $f(T)(Y) < 0$. Therefore $f(S) \neq f(T)$ and f is injective.

There exists a well known bound on $|T_n^1|$:

$$|T_n^1| \leq 2 \sum_{i=0}^n \binom{2^n - 1}{i} \leq 2^{n^2}.$$

This combined with Proposition 5.1 yields an upper bound for $|T_n^d|$ and $|\bar{T}_n^d|$. Yet this can be strengthened using the following extension of a result of Cameron and Winder.

Theorem 5.2:

Let m, f, n be three positive integers such that $f \leq n$. Let

$B_{f,n}^m$ be the maximum number of regions that m hyperplanes corresponding to m linear equations in the same f variables determine in \mathbb{R}^n . Then:

$$(1) B_{f,n}^m = B_{f,f}^m$$

$$(2) \text{ if we write } B_f^m \text{ for } B_{f,f}^m \text{ then: } B_f^m = 2 \sum_{i=0}^{f-1} \binom{m-1}{i}$$

Proof: (1) The projection: $(x_1, \dots, x_f, x_{f+1}, \dots, x_n) \rightarrow (x_1, \dots, x_f)$ of \mathbb{R}^n into \mathbb{R}^f establishes a one to one correspondence between regions of the two spaces.

(2) is obtained by solving the simple recurrence relation:

$$B_f^m = B_f^{m-1} + B_{f-1}^{m-1}.$$

We remark now that to every vertex X of H^n we can attach a linear form $\ell_X: F_n(\mathbb{R}) \rightarrow \mathbb{R}$ with $\ell_X(P) = P(X)$.

In particular if $|I| = f$, assimilating $T_n^I(\mathbb{R})$ to a subset of \mathbb{R}^f , every point X of H^n yields a linear form $\ell_X: \mathbb{R}^f \rightarrow \mathbb{R}$. Each hyperplane $\ell_X = 0$ separates \mathbb{R}^f and hence $T_n^I(\mathbb{R})$ into two regions. There are 2^n such hyperplanes. Therefore:

Proposition 5.3:

$$|T_n^I| \leq B_{|I|}^{2n} = 2 \sum_{k=0}^{|I|-1} \binom{2n-1}{k}.$$

We have the simple estimates:

$$|T_n^I| < 2 |I| \binom{2n-1}{|I|-1} \text{ for } |I| \leq \frac{2n+1}{2}$$

and then:

$$|T_n^I| < (2^n - 1)^{|I|-1} \text{ if in addition } \frac{2|I|}{|I|-1} \leq 1$$

i.e. if $|I| \geq 5$. Several bounds can be obtained using these estimates. In particular we have:

Theorem 5.4:

$$(1) |\bar{T}_n^d| < 2 \frac{n^{d+1}}{d!} \quad \text{as soon as } \binom{n}{d} \geq 5$$

$$(2) |\bar{T}_n^d| < 2 \frac{n^{d+1}}{(d-1)!} \quad \text{as soon as } r(n,d) \geq 5 \text{ and } d \leq \lfloor \frac{n}{2} \rfloor$$

Proof: Apply Proposition 5.3 and the corresponding simple estimates with $|I| = \binom{n}{d}$ for (1) and $|I| = r(n,d)$ for (2).

These bounds are tight for small values of d and deteriorate when d increases. Using the symmetry of homogeneous forms (i.e. 2^{n-1} hyperplanes instead of 2^n) does not improve the bound $2^{n^{d+1}}$. Notice also that there exists essentially a one to one correspondence between homogeneous forms of degree d and $n - d$:

$$\text{if } P_n^d = \sum_{|I|=d} a_I x^I \quad \text{define} \quad Q_n^{n-d} = \sum_I a_I x^{N-I}.$$

Therefore we expect:

$$|\bar{T}_n^d| = |\bar{T}_n^{n-d}|, |\bar{A}_n^d| = |\bar{A}_n^{n-d}| \dots$$

We now prove the following:

Theorem 5.5: For $1 \leq d \leq n$:

$$(1) |A_n^1| = |\bar{A}_n^1| = 2^n.$$

$$(2) |\bar{A}_n^d| < 2 \frac{n^{d+1}}{(d-1)!} \quad \text{for } \binom{n-1}{d-1} \geq 5.$$

$$(3) |A_n^d| < 2 \frac{n^{d+1}}{(d-2)!} \quad \text{for } r(n-1,d-1) \geq 5 \text{ and } d \leq \lfloor \frac{n+1}{2} \rfloor.$$

$$(4) |A_n^n| < 2^n 2^{n-1}.$$

Proof: (1) This is clear since the orientation of any edge parallel to the i -th coordinate axis depends only on the sign of $\alpha_{\{i\}}$. Notice that this enumeration is for linear forms such that $\alpha_{\{i\}} \neq 0$ for any i . These are the only linear forms which define properly an A.O. of H^n which in addition belongs to $G(H^n)$ since the minimum is also global. If one allows 0 coefficients in the form then some ambiguities arise in the orientations of corresponding edges and we then have a more general bound of 3^n .

(2) is similar to (3).

(3) Given a neural network with energy in F_n^d , recall that every neuron simulated an algebraic threshold function in T_{n-1}^{d-1} . Therefore:

$$|A_n^d| \leq |T_{n-1}^{d-1}|^n.$$

Using theorem 5.4:

$$|A_n^d| < \left[2^{\frac{n^d}{(d-2)!}} \right]^n = 2^{\frac{n^{d+1}}{(d-2)!}}.$$

(4) The total number of orientations (including cyclic ones) is $2^{|E|} = 2^n 2^{n-1}$. This bound can be microscopically improved, for instance, by deducting the number of cyclic orientations where a given fixed face receives a cyclic orientation.

Because of (4) the bounds in (2) for instance is interesting iff:

$$\frac{n^{d+1}}{(d-1)!} \leq n 2^{n-1} \text{ or } n^d \leq (d-1)! 2^{n-1}$$

We turn now to lower bounds. The threshold functions corresponding to the different neurons are obviously dependent. Yet, as in [Abu Mostafa, St.Jacques,1985] for $d \leq \lfloor \frac{n}{2} \rfloor$ we can study the collection of networks where the first

$\lfloor \frac{n}{2} \rfloor$ neurons simulate independent threshold functions of degree $d - 1$ in the remaining $\lfloor \frac{n}{2} \rfloor$ variables. Since here we are mainly interested in asymptotic values, we shall not distinguish the cases: n even or odd. Such a distinction leads only to Lilliputian improvements. We know that in some sense: $T_n^I \subset T_{\lfloor \frac{n}{2} \rfloor - 1}^1$ and in [Muroga, Toda, 1966] a construction shows that:

$$|T_n^1| > 2^{\frac{n(n-3)}{2} + 8} \text{ for } (n \geq 9)$$

Yet, we cannot use it here for $d > 2$, because the inclusion above is strict. For the special important case of $d = 2$ we get:

$$\left(2^{\frac{\lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor - 3) + 8}{2}} \right)^{\lfloor \frac{n}{2} \rfloor} < |A_n^2| < 2^{n(n-1)^2}$$

hence the capacity C_n^2 is exactly of the order of n^3 bits. However, the following is true:

Theorem 5.6:

$$|T_n^I| > 2^{|I|}$$

Proof: Consider the square matrix M with

-2^n rows indexed by the vertices $X = (x_1, \dots, x_n)$ of H^n

-2^n columns indexed by the subsets I of $N = \{1, 2, \dots, n\}$

and such that: $M(X, I) = x^I = \prod_{i \in I} x_i$ ($x^\emptyset = 1$).

It can be shown that M is a Hadamard matrix and therefore $\det M \neq 0$. In particular for any set $I \subset P(N)$ we can find $|I|$ vectors on H^n such that the corresponding $|I| \times |I|$ submatrix has full rank. Let M_I be such a matrix, corresponding to vectors $Y_1, Y_2, \dots, Y_{|I|}$ of H^n . If $\alpha = (\alpha_I)$ is the column vector representing the coefficients of an element in F_n^I , the system: $M_I \alpha = \beta$ has a unique solution for any vector β . In particular for any subset A of

$\{1, 2, \dots, |I|\}$ we can find an element T in T_n^I such that: $T(Y_i) > 0$ if $i \in A$ and $T(Y_i) < 0$ if $i \in \{1, 2, \dots, |I|\} - A$.

Therefore, $2^{|I|} < |T_n^I|$.

As a straightforward application: $|T_n^d| > 2^{\binom{n}{d}}$ and

$|T_n^d| > 2^{r(n,d)}$. Because of $|A_n^d| > |T_{\lfloor \frac{n}{2} \rfloor}^{d-1}|$, and of

$|\bar{A}_n^d| > |\bar{T}_{\lfloor \frac{n}{2} \rfloor}^{d-1}|$, we have:

Theorem 5.7:

For $d \leq \lfloor \frac{n}{2} \rfloor$: $|\bar{A}_n^d| > 2^{\binom{\lfloor \frac{n}{2} \rfloor}{d-1} \lfloor \frac{n}{2} \rfloor}$ and

$$|A_n^d| > 2^{r(\lfloor \frac{n}{2} \rfloor, d-1) \lfloor \frac{n}{2} \rfloor}.$$

Using simple bounds in these exponents yields:

$$|A_n^d| > 2^{\frac{1}{(d-1)!} \lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor - d + 2)^{d-1}} \text{ and also}$$

$$|A_n^n| > |A_{\lfloor \frac{n}{2} \rfloor}^{\lfloor \frac{n}{2} \rfloor}| > 2^{\lfloor \frac{n}{2} \rfloor \left(2^{\lfloor \frac{n}{2} \rfloor} - 1 \right)}.$$

Let C_n^d be the capacity of the algebraic forms of degree d on H^n , and C the total capacity of H^n . Then we can sum part of our results in:

Theorem 5.8:

For $d \leq \lfloor \frac{n}{2} \rfloor$:

$$\frac{1}{(d-1)!} \lfloor \frac{n}{2} \rfloor (\lfloor \frac{n}{2} \rfloor - d + 2)^{d-1} < C_n^d < \frac{n^{d+1}}{(d-2)!} \text{ and}$$

$$\lfloor \frac{n}{2} \rfloor (2^{\lfloor \frac{n}{2} \rfloor} - 1) < C < n 2^{n-1}.$$

VI. STABLE STATES

The discrete neural network presented in the introduction can be used as a model of associative content-addressable memory capable of storing and processing information; the storage is made in a certain subset of the local minima of the energy function E on H^n and the processing occurs during the evolution of the network as error correction and nearest neighbor search.

We shall now:

(1) introduce a general formula for the storage of stable states in a network with E in \bar{F}_n^d , show its invariance under the action of a group of isometries and a new explanation for the appearance of additional stable states in many situations.

(2) derive a general bound, independent of the storage rule adopted, for the maximal number of arbitrarily chosen points that can be made stable.

(3) study possible alternatives in the case $d = 2$.

(4) analyze in some details the properties of networks in which orthogonal states have been stored.

Throughout this chapter we shall assume, for simplicity, that all thresholds are set to 0.

(1) Outerproduct formula of degree d - Action of isometries.

In order to store k vectors "or memories" M^1, \dots, M^k of H^n as stable states of a form of degree d we introduce the homogeneous energy function:

$$E(X) = \frac{-1}{d!} \sum_{|I|=d} \sum_{i=1}^k M_I^i x^I \quad \text{where}$$

$$M_I^i = \prod_{j \in I} M_j^i \quad \text{and} \quad M^i = (M_1^i, \dots, M_n^i) .$$

This is a generalization of the classical outerproduct scheme or Hebb's rule where $d = 2$, and we shall call it: outerproduct scheme of degree d .

The appropriateness of such a construction can be seen using the same simple statistical considerations as in [Hopfield,1982]. Insight can also be obtained from the special case where the vectors M^1, \dots, M^k are orthogonal. We present here an additional point of view in favor of this formula which is helpful also in other considerations.

A one to one map $\sigma: H^n \rightarrow H^n$ will be called an isometry iff it preserves the Hamming distance between points. The set of all such isometries is a group I_n which is a subgroup of the group of isometries of \mathbb{R}^n with the euclidean distance, and which is generated by two kinds of isometries:

- σ_{ij} which permutes the i and j coordinates
- the inversion $\tau(X) = \tau(-X)$.

It is also the set of all $n \times n$ matrices with $n - 1$ zeros in each row and column, the non zero entry in each line being -1 or $+1$ and as such is called the monomial group. Alternatively it can be seen as the wreath product: $\mathbb{Z}_2 \otimes_w S_n$. In any case $|I_n| = 2^n \times n!$. Two orientations of H^n will be said isometric iff there exists an isometry of H^n sending one orientation into the other. The following theorem shows that the outerproduct scheme behaves very nicely with respect to isometries.

Theorem 6.1:

Let M^1, \dots, M^k be in H^n . Let σ be any isometry in I_n . Let E (resp. E^σ) be the form in $\bar{F}_n^d(\mathbb{R})$ obtained by the outerproduct scheme of degree d applied to the vectors M^ℓ (resp. $\sigma(M^\ell)$) $\ell = 1, \dots, k$. Then, for any vertex X of H^n ,

$$E(X) = E^\sigma(\sigma(X)) .$$

Proof: (We shall omit a few simple algebraic steps.)

It is enough to show it for the generators of I_n .

1st case: $\sigma = \tau$. Then:

$$E^\sigma(\sigma(X)) = - \frac{1}{d!} \sum_{|I|=d} \sum_{i=1}^k (-1)^d M_I^i (-1)^d x^I = E(X)$$

2nd case: $\sigma = \sigma_{ab}$. Then:

$$\begin{aligned} E^\sigma(\sigma(X)) &= - \frac{1}{d!} \sum_{|I|=d} \sum_{i=1}^k (\sigma_{ab} M^i)_I x^{\sigma_{ab}(I)} = \\ &= - \frac{1}{d!} \sum_{|I|=d} \sum_{i=1}^k M_{\sigma_{ab}(I)}^i x^{\sigma_{ab}(I)} = E(X). \end{aligned}$$

Since the values assumed by the energy function entirely define an A.O. of H^n , Theorem 6.1 shows that the outerproduct scheme is invariant under the action of the group I_n . But there is a deeper consequence to theorem 6.1. If H denotes the subgroup of I_n that leaves the set $\{M^1, \dots, M^k\}$ globally invariant then for any h in H and any X in H^n we have:

$$E(X) = E^h(h(X)) = E(h(X))$$

Moreover, any isometry h preserves the neighborhood relations. Therefore, if X is a stable point, so is the entire

orbit $H(X)$. The action of H partitions the hypercube H^n into orbits of equal energy, each one being characterized by a common dynamical behavior of its points. This property, as we shall see, can be used in counting stable states and accounts for their great number.

[In the case where d is even it is easy to see that the inversion τ should be included in H .]

(2) General bound on storage:

It is known, that in order to use the outerproduct scheme effectively, k should not be "too large" and the vectors M^1, \dots, M^k should not be "too correlated". When $d = 2$, Hopfield predicted experimentally a maximal storage capacity of the order: $k \approx 0.15n$, and in [McEliece, Posner, Rodemich, Venkatesh, 1986] a statistical bound of $\frac{n}{2 \log n}$ can be found. Similar results can be obtained for $d > 2$ [Baldi, Venkatesh, 1986]. Nevertheless these estimates are restricted to the outerproduct construction. The following natural question arises: for any fixed d , what is the maximum k such that any k vectors of H^n can be made stable in a generalized neural network with energy function in $F_n^d(\mathbb{R})$?

We have the theorem:

Theorem 6.2:

Suppose that for any k vectors M^1, \dots, M^k of H^n we can find a form Q in $F_n^d(\mathbb{R})$ such that M^1, \dots, M^k are local minima of Q on H^n . Then:

$$k \leq r(n-1, d-1) = \sum_{i=0}^{d-1} \binom{n-1}{i}$$

Proof: We generalize the proof of the case $d = 2$ in [Abu-Mostafa and St. Jacques, 1985].

Consider k vectors M^1, \dots, M^k . Fix their $n-1$ last coordinates

such that they are all different ($k < 2^{n-1}$). Consider the threshold function corresponding to the first generalized neuron i.e. to the first coordinate. For any of the 2^k possible choices for M_1^1, \dots, M_1^k we must find an algebraic form Q in F_{n-1}^{d-1} such that:

$$\text{sgn}(Q(M_2^i, \dots, M_n^i)) = M_1^i \quad i = 1, \dots, k.$$

For any i the coefficients M_2^i, \dots, M_n^i define an hyperplane in the space F_{n-1}^{d-1} . There are k such hyperplanes and we have seen they determine at most $B_{r(n-1, d-1)}^k$ regions. Therefore:

$$2^k \leq 2^{\sum_{i=0}^{r(n-1, d-1)-1} \binom{k-1}{i}}.$$

If $k > r(n-1, d-1)$ then we should have:

$$2^k < 2^{\sum_{i=0}^{k-1} \binom{k-1}{i}} = 2^k \quad \text{a contradiction.}$$

So:

$$k \leq r(n-1, d-1).$$

(3) Other formulas for $d = 2$:

The outerproduct rule is by no means the only possible one. For several applications it is reasonable to require for any sensible formula to be:

(i) invariant under the action of I_n

(ii) local in the sense that deletion or addition of a new memory M^1 should be possible via simple independent computations on subsets of components of M^1 of size at most d if a form in F_n^d is to be used. If $d = 2$ and if we let M be the

$n \times k$ matrix whose columns are the vectors M^1, \dots, M^k then the outerproduct rule leads to the energy function: $E(X) = -\frac{1}{2} X^T A X$ where: $A = M M^T - kI$ is the symmetric, 0-diagonal matrix of synaptic interconnections between neurons. A can also be written as: $A = \sum_{i=1}^k M^i M^{iT} - kI$. There exist many situations where different importance is attached to the different states one wants to recall. This leads to the following possible generalization: attach a positive weight λ_i to each M^i and define the connection matrix to be:

$$A = \sum_{i=1}^k \lambda_i M^i M^{iT} - \Lambda I$$

where $\Lambda = \sum_{i=1}^k \lambda_i$. In matrix notation A can also be written:

$A = (MD)(MD)^T - \Lambda I$ where D is a diagonal $k \times k$ matrix, with elements $\sqrt{\lambda_i}$ on the diagonal. In the next section we shall study the effect of the introduction of the weights λ_i on the A.O. of H^n . This weighted outerproduct formula can easily be extended to networks with energy function in F_n^d , $d > 2$, and satisfies the two requirements (i) and (ii).

When the vectors M^i are orthogonal the matrix $\frac{1}{n} M M^T$ describes the orthogonal projection onto the space $\langle M^i, i=1, \dots, k \rangle$. Based on this remark, Personnaz, Guyon and Dreyfus have introduced another alternative to the Hebbian rule for $d = 2$, called the "projection rule". They use a neural network with a synchronous updating scheme, i.e. all the neurons are updated at the same time and in parallel at each step. The synchronous scheme is deterministic and always converges to a stable state or to a cycle. If the matrix of interconnections is symmetric it can be shown that all cycles have length at most 2. In the general case, longer cycles can be obtained.

To define the "projection rule" let M^I be the Moore-Penrose

pseudoinverse of M . Let $A = MM^I$ and $E(X) = -\frac{1}{2}X^TAX$. Then A is the matrix of the orthogonal projection onto the space $\langle M^i, i=1, \dots, k \rangle$ and it can be shown that in this special case the network, if updated synchronously, always converges to a stable state. Indeed, given a point X on H^n , the system first projects X orthogonally onto $\langle M^i, i=1, \dots, k \rangle$ and then by the thresholding operation, selects the point of H^n closest to $A(X)$. A vector X is stable iff it is the closest vector of H^n to its projection. Because of this geometric interpretation, the "projection rule" is also invariant under the action of I_n . In the analysis of stable states, even a larger group H can be taken, for if X is stable and α is an isometry leaving $\langle M^i, i=1, \dots, k \rangle$ globally invariant, then A and A^α are the same operator and therefore $\alpha(X)$ must be also stable.

(4) Orthogonal case:

We restrict now ourselves to the case where M^1, \dots, M^k are orthogonal, $d = 2$, and the matrix A is given by the weighted outerproduct formula:

$$A = \sum_i \lambda_i M^i M^{iT} - \Lambda I .$$

Special attention will be given to the usual case: $\lambda_i = 1$. It is easy to see that we have:

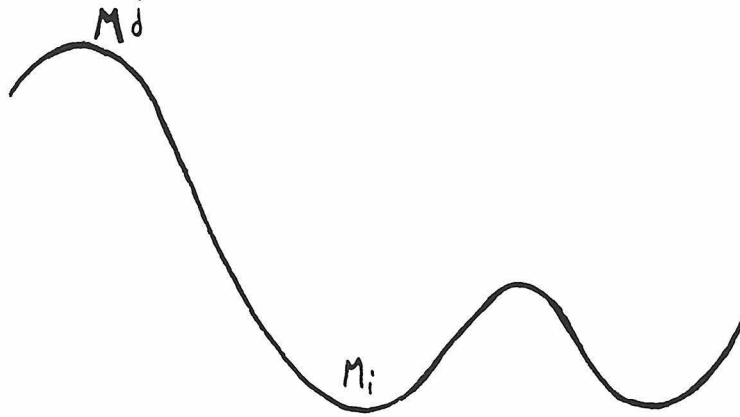
$$A(M^i) = (n\lambda_i - \Lambda)M^i \text{ and } E(M^i) = -\frac{1}{2} n(n\lambda_i - \Lambda)$$

for $i = 1, \dots, k$. Also for any M^j in H^n orthogonal to $\langle M^i, i=1, \dots, k \rangle$ (if it exists) we have:

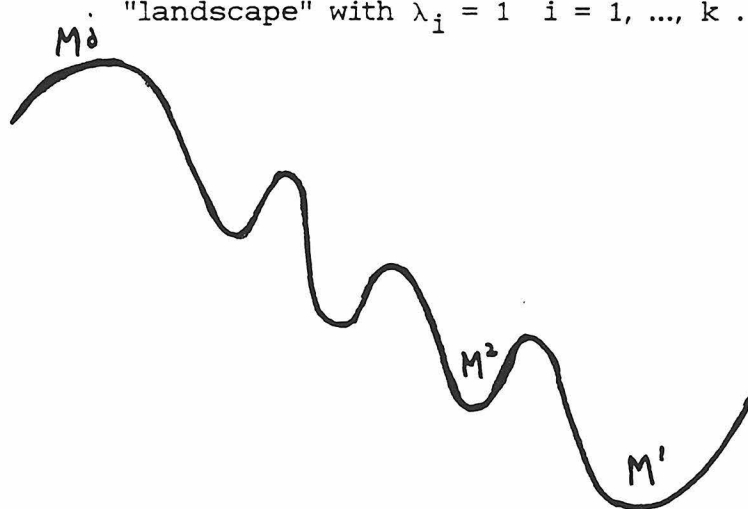
$$A(M^j) = \Lambda M^j \text{ and } E(M^j) = \frac{1}{2} n \Lambda .$$

If $n\lambda_i - \Lambda \geq 0$ then M^i and $-M^i$ are stable states of the corresponding network. Moreover the energy of M^i is proportional to $n\lambda_i - \Lambda$. Because of the elementary properties of real symmetric matrices and associated quadratic forms the memory with the highest weight λ_i will

yield a minima of the energy on the sphere of radius \sqrt{n} and therefore also on H^n . Any M^j orthogonal to $\langle M^i, i=1, \dots, k \rangle$ corresponds to a maxima of the energy and therefore to a highly unstable point. The weights λ_i deform the depth of the "valleys".



"landscape" with $\lambda_i = 1 \quad i = 1, \dots, k$.



"landscape" with $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_k$.

We turn now to the size of the basins of attraction. If X is a vector of H^n and if d_i is the Hamming distance from X to M^i then:

$$A(X) = \sum_{i=1}^k \lambda_i (n - 2d_i) M^i - \Lambda X$$

$$E(X) = \frac{1}{2} X^T \Lambda X - \frac{1}{2} \sum_{i=1}^k \lambda_i (n-2d_i) X^T M^i$$

Because of the orthogonality of the memories, the triangle inequality on the Hamming distance and the invariance under the action of I_n we have the following properties for the distances d_i $i = 1, \dots, k$:

(i) without loss of generality we can assume $d_i \leq \frac{N}{2}$
(otherwise replace M^i by $-M^i$)

(ii) for any i and ℓ $d_i + d_\ell \geq \frac{N}{2}$ and the inequality
is strict for $X \neq M^i, X \neq M^\ell$

(iii) if we reorder M^1, \dots, M^k so that $d_1 \leq d_2 \leq \dots \leq d_k$ then:

$$d_i \leq \frac{N}{2} - d_1 \quad 2 \leq i \leq k$$

$$(iv) \quad d_i \geq \frac{N}{4} \quad 2 \leq i \leq k$$

$$(v) \quad d_1 \geq \frac{N}{2} - d_i \geq \frac{N}{2} - d_k$$

$$(vi) \quad \text{if } d_1 = d_i = d_k \text{ then } d_i \geq \frac{N}{4} \quad 1 \leq i \leq k$$

Assume now that X is our starting state and we ask under which condition on d_1 can we be certain that the system will converge to M^1 ? By using again the invariance of the dynamical behavior under the action of I_n we can assume without loss of generality that: $M^1 = (1,1,\dots,1)^T$ and $X = (-1,-1,\dots,-1,1,\dots,1)^T$. Since:

$$A(X) = \lambda_1(N-2d_1) + \sum_{i=2}^k \lambda_i(N-2d_i)M^i - \Lambda X$$

we see that if X is to converge M^1 we must have:

$$\lambda_1(n-2d_1) + \sum_{i=2}^k \lambda_i(n-2d_i)M_j^i + \Lambda > 0 \quad 1 \leq j \leq d_1$$

$$\lambda_1(n-2d_1) + \sum_{i=2}^k \lambda_i(n-2d_i)M_j^i - \Lambda \geq 0 \quad d_1 < j \leq n.$$

In both inequalities, the worst case occurs when $\sum_{i=2}^k \lambda_i(n-2d_i)M_j^i$ is minimal. Because of inequality (iii) above we have:

$$\sum_{i=2}^k \lambda_i(n-2d_i)M_j^i \geq - \sum_{i=2}^k \lambda_i 2d_i = -2d_1(\Lambda - \lambda_1).$$

Substituting in both inequalities we finally get:

$$d_1 \leq \frac{n\lambda_1 - \Lambda}{2\Lambda}.$$

It is easy to construct examples of small size where this bound is attained; as a general bound it is best possible. Therefore the radius of the basin of attraction (as well as their depth) is affected by the weights λ_i . We have:

Theorem 6.3:

In a neural network corresponding to a weighted outerproduct on k orthogonal vectors M^1, \dots, M^k with weights $\lambda_1, \dots, \lambda_k$ if $n\lambda_i - \Lambda \geq 0$ then M^i is a stable state and its radius of attraction R_i satisfies:

$$\left\lfloor \frac{n\lambda_1 - \Lambda}{2\Lambda} \right\rfloor \leq R_i.$$

In the usual case $\lambda_i = 1$, we have:

$$\left\lfloor \frac{n-k}{2k} \right\rfloor \leq R_i.$$

In the previous drawings of the landscape of the energy on H^n we did not include an essential fact: in the general case there exist additional stable states in the systems which are not in the set $\{\pm M_i: i=1, \dots, k\}$. We shall briefly study these states using the action of I_n . In the weighted outerproduct formula, the interesting subgroup H is the subgroup of I_n leaving $\{\pm M_i, i=1, \dots, k\}$ globally invariant. For simplicity we shall assume for the rest of this chapter that $\lambda_i = 1 \quad i=1, \dots, k$. In this case $\frac{1}{n}MM^T$ is the matrix of the orthogonal projection onto $\langle M_i, i=1, \dots, k \rangle$. Therefore, we can take for H the subgroup of I_n leaving the linear space $\langle M_i, i=1, \dots, k \rangle$ globally invariant.

Let X be a state such that $d_i = d(X, M^i) < \frac{n}{2}$. Then, since the vectors M^i have the lowest energy levels we must have: $n^2 \geq \sum_{i=1}^k (n-2d_i)^2$. In particular if $d_i = d \quad i = 1, \dots, \ell$ and $d_i = \frac{n}{2} \quad i = \ell + 1, \dots, k$ then:

$$n^2 > \ell (n-2d)^2 \quad \text{or} \quad \frac{n}{2} \frac{\sqrt{\ell}-1}{\sqrt{\ell}} < d .$$

For such an X we have: $A(X) = \sum_{i=1}^{\ell} (n-2d)M^i - kX$ and X is stable iff:

$$(n-2d) \sum_{i=1}^{\ell} M_j^i X_j \geq k \quad j = 1, \dots, n .$$

Therefore, if X is to be stable we must have: $X_j = \text{sgn}(\sum_{i=1}^{\ell} M_j^i)$.

In particular $\sum_{i=1}^{\ell} M_j^i$ must be nonzero which is always

the case for ℓ odd. If $\sum_{i=1}^{\ell} M_j^i = 0$ for any j then the

condition $\frac{n-k}{2} \geq d$ is sufficient to ensure stability of X .

Notice also that X is not in the basin of attraction of any

M^i , therefore we also have: $d > \frac{n-k}{2k}$. In summary:

Proposition 6.4:

Consider a neural network corresponding to an outerproduct formula on k orthogonal vectors M^1, \dots, M^k of H^n . Let S be a non empty subset of $\{1, \dots, k\}$ such that: $\sum_{i \in S} M_j^i \neq 0$ for any $j = 1, \dots, n$. Let X be such that $X_j = \text{sgn} \sum_{i \in S} M_j^i$. If $d(X, M^i) = d$ for i in S , and $d(X, M^i) = \frac{n}{2}$ for i not in S , then a sufficient condition for the stability of X is: $d \leq \frac{n-k}{2}$.

Under these assumptions d shall also satisfy:

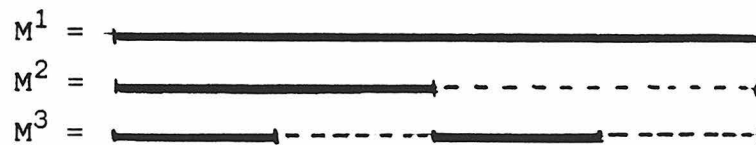
$$\max \left[\frac{n-k}{2k}, \frac{n(\sqrt{|S|} - 1)}{2\sqrt{|S|}} \right] < d .$$

As a simple application we can state:

Theorem 6.5:

In a neural network corresponding to an outerproduct formula on k orthogonal vectors of H^n , the number of stable states is: 2 for $k = 1$, 4 for $k = 2$, and 14 for $k = 3$.

Proof: Case $k = 1, 2$: left as an exercise. Case $k = 3$: notice that n must be a multiple of 4. By using the invariance of the dynamical behavior under the action of I_n we can assume without loss of generality that:



The majority vector X



satisfies the condition of Proposition 6.4. Therefore $\{\pm M_i, \pm X\}$ are all stable states. By writing up the conditions for stability it is easy to see that the coordinates of any stable vector must have a constant sign in each one of the

four "quarters". There are at most $2^4 = 16$ stable states. The group H which leaves $\langle M^1, M^2, M^3 \rangle$ globally invariant contains the isometries $\tau, \alpha_1, \alpha_1^*, \alpha_2, \alpha_2^*$ where:

$-\tau$ is the multiplication by -1 :

$-\alpha_1$ is the cyclic shift of length $\frac{n}{2}$:

$$\alpha_1(X) = \text{—————} \text{-----} \text{—————}$$

$-\alpha_1^*(X)$ is the symmetry with respect to the central axis:

$$\alpha_1^*(X) = \text{-----} \text{—————} \text{-----}$$

$-\alpha_2$ is the cyclic shift of length $\frac{n}{4}$ on the first and last $\frac{n}{2}$ bits separately

$$(\alpha_2(X) = \text{—————} \text{-----} \text{—————})$$

$-\alpha_2^*$ is the symmetry with respect to the quarter axis on the first and last $\frac{n}{2}$ bits separately

$$\alpha_2^*(X) = \text{—————} \text{-----} \text{—————}$$

Therefore we have 14 stable states:

$$\{\pm M^1, \pm M^2, \pm M^3, \pm X, \pm \alpha_1(X), \pm \alpha_1^*(X), \pm \alpha_2(X)\} .$$

In this case, the orbit of X under H yields all the additional stable states, for it is easy to check that the remaining candidate Y :

$$Y = \text{—————} \text{-----} \text{—————}$$

and its opposite are unstable since they are orthogonal to M^1, M^2 and M^3 .

To finish this chapter let us mention an interesting, partially open problem. It is a well known fact that in diverse occasions the output of biological systems seems to be invariant under the action of a certain group. It is the case in perception, in vision for instance, where objects can be recognized in spite of several types of deformations. This motivates the following question: given a group G acting on

H^n can we find an energy function (and hence a neural network) "corresponding" to G . For instance, is there a form in F_n^d which takes a constant different value on each orbit of G or one such that if X is stable so is $G(X)$ at least for a carefully chosen subset of vectors X ? In particular, which groups can be represented in such a fashion using only quadratic forms?

VII. SOME STATISTICAL PROPERTIES

It is of interest to introduce probability distributions on the previously studied sets. The easiest case corresponds to the introduction of uniform distributions $U_n(S)$ on the various sets: $L(G)$, $A_n^d(G)$...

Some simple computations can be done at least in the case of $U_n(L(H^n))$ where any linear ordering of the vertices is equiprobable with probability $\frac{1}{2^{n!}}$.

As in [Harary,1972] define the indegree (resp. outdegree) of a point to be the number of vertices adjacent to (resp. from) it. A point basis is a minimal collection of points from which all vertices are reachable. It is known that every acyclic digraph has a unique point basis consisting of all vertices of indegree 0. Vertices of outdegree 0 are the stable points. Point basis correspond to "valleys":

Theorem 7.1:

With the distribution $U_n(L(H^n))$:

average number of stable points = $\frac{2^n}{n+1}$ = average size of a point basis.

Proof: There exists an obvious symmetry between points of indegree 0 and points with outdegree 0. The average is given by:

$$\frac{2^n}{2^{n!}} \sum_{k=n+1}^{2^n} n! \binom{k-1}{n} (2^{n-n-1})! = \frac{2^n}{n+1} .$$

In [Tovey,1985] a proof is given of:

Theorem 7.2:

With the distribution $U_n(1(H^n))$, the expected number of iterations of the local algorithm is less than $\frac{3}{2} \ln n$.

VIII. COMPLEXITY AND REDUCTION ALGORITHM

The theory of neural networks has an obvious origin in neurobiology and natural applications to circuit architectures. Conceptually, one way they have been considered is from the standpoint of error corrections and content-addressable memory (CAM). However, we have seen that the basic operation performed even by the generalized neural networks is the search for the local minima of an algebraic energy function. Therefore a second approach becomes possible in a context of optimization problems, which leads us to the following question: how difficult and how fundamental is it to find the minimum of an algebraic form over the hypercube H^n ?

This approach is not new and several results are already known (for instance [Hopfield,Tank,1985]). A few of them arose first in statistical mechanics in the theory of spin glasses. This is no wonder since neural networks can be interpreted as a certain limiting form of spin glasses and important relations between statistical mechanics and combinatorial optimization problems have been discovered in the past years [Kirkpatrick,Gelatt,Vecchi,1983]. As a result new ways of dealing with traditionally intractable problems have appeared (for example: simulated annealing).

We shall now try to organize a few complexity results in terms of neural networks including some extensions and simplifications. Denote by $\text{Min } Q, Q \in F_n^d(A)$ the general problem of minimizing a form Q in $F_n^d(A)$ over the hypercube H^n . Recall that if the decision problem "Is there a point X such that $Q(X) < K$?" is NP complete the corresponding optimization problem is NP hard. Also, in order to have problems with finite input, we shall require A to be a subset

of the integers. We have the following:

Theorem 8.1:

Min Q , Q in $F_n^d(\mathbb{Z})$ or $\bar{F}_n^d(\mathbb{Z})$ is NP hard for $d > 1$ and is in P for $d = 1$.

Proof: (1) If $d = 1$ let $Q(X) = x_0 + \sum_1^n a_i x_i$. Then the minimum of Q is attained for $X = (-\text{sgn } a_1, \dots, -\text{sgn } a_n)$.

(2) We shall first show that: if Min Q , Q in $F_n^{d'}(\mathbb{Z})$ or $\bar{F}_n^{d'}(\mathbb{Z})$ is in P then Min Q , Q in $F_n^d(\mathbb{Z})$ or $\bar{F}_n^d(\mathbb{Z})$ is also in P for $d < d'$. The proof is by induction.

If $Q \in F_n^d(\mathbb{Z})$ (resp $\bar{F}_n^d(\mathbb{Z})$) then if y is an additional variable the form $Q' = yQ$ is in $F_{n+1}^{d+1}(\mathbb{Z})$ (resp. $\bar{F}_{n+1}^{d+1}(\mathbb{Z})$). Assume that we have a polynomial time algorithm for forms in $F_n^{d+1}(\mathbb{Z})$ and hence for forms in $\bar{F}_{n+1}^{d+1}(\mathbb{Z})$. Apply this algorithm to Q' . $m' = \text{Min } Q' = \text{Min}(\text{Min } Q, \text{Min } -Q) = \text{Min}(\text{Min } Q, -\text{Max } Q)$.

1st case: m' is attained for $y = +1$. Then $m' = \text{min } Q$.

2nd case: m' is attained for $y = -1$. Then $m' = -\text{max } Q$.

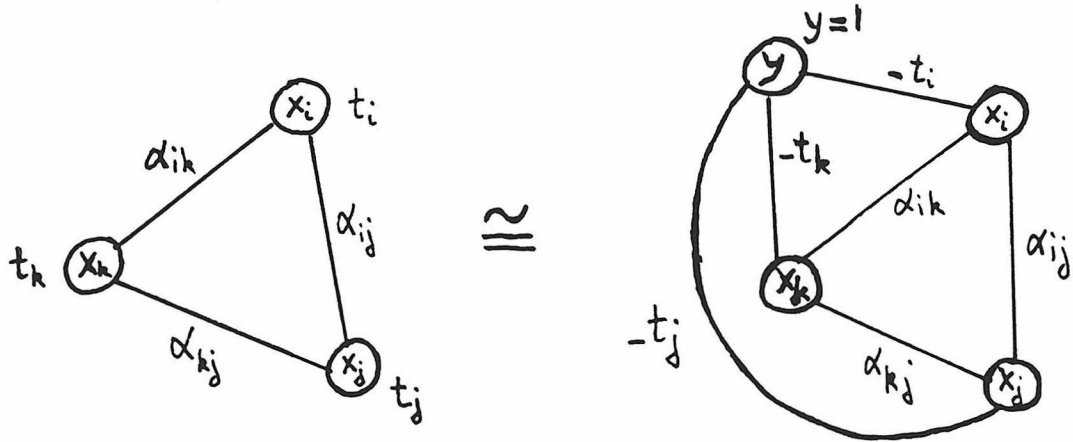
Consider $Q'' = y(Q+m')$. Then Q'' is in $F_{n+1}^{d+1}(\mathbb{Z})$ and:

$m'' = \text{Min } Q'' = \text{Min}(\text{Min } Q+m', -\text{Max } Q-m') = \text{Min}(\text{Min } Q+m', 0) = \text{Min } Q + m'$ and so $\text{Min } Q = m'' - m'$.

Therefore we can restrict ourselves to quadratic forms. It is not difficult to see that a large variety of NP complete problems can be encoded very easily into quadratic form optimization. An example using a reduction from TSP (Traveling Salesman Problem) can be found in [Hopfield, Tank, 1985]. It is in fact the easiness of such an encoding in many instances, rather than its existence in one of them, that is important to us. We shall give here a slightly different proof that yields some additional information. First of all, notice that we can restrict ourselves to the problem $\text{Min } Q$, Q in $\bar{F}_n^2(\mathbb{Z})$. Indeed,

if $Q = \sum_{i,j} \alpha_{ij} x_i x_j + \sum_i \alpha_i x_i + \alpha_0$ consider the form

$Q' = \sum_{i,j} \alpha_{ij} x_i x_j + \sum_i \alpha_i x_i y$ in $\bar{F}_{n+1}^2(\mathbb{Z})$, where y is some additional variable. Because of its symmetry, Q' reaches its minimum for a point on H^{n+1} where $y = +1$. This point yields a minimum for Q . The algebraic operation of introducing the variable y has an interesting interpretation from the point of view of the neurons. Given a neural network with energy function: $E(X) = -\frac{1}{2} \sum_{i,j} \alpha_{ij} x_i x_j + \sum_{i=1}^n t_i x_i$ it is completely equivalent to a network with $n + 1$ neurons with 0 thresholds, the new additional neuron y being connected to each neuron x_i with an edge of weight $-t_i$. In addition, y must be held to the value $+1$.



Thresholds can therefore be suppressed by increasing the complexity of the graph G of interconnections. Now $\text{Min } Q, Q$ in $\bar{F}_n^2(\mathbb{Z})$ is trivially equivalent to the NP hard problem "Matrix Cover" [Garey,Johnson,1979] and stays so even if the symmetric matrix (α_{ij}) is required to be positive definite.

Biological hardware seem to perform operations that are more of a "matching" type rather than boolean or arithmetic. It is therefore interesting also to investigate further the relation between our discrete optimization problem and questions of the matching type. For this purpose consider the

restricted problem $\text{Min } Q, Q \text{ in } \bar{F}_n^2(\mathbb{Z}^+)$. Write Q as an energy function:

$$Q(X) = -\frac{1}{2} \sum_{i,j} a_{ij} \quad \text{where } a_{ij} \leq 0.$$

If we let $k = \sum_{i,j} a_{ij}$ with the obvious notations we have:

$$Q(X) = -\frac{1}{2}(k - 2 \sum_{\substack{i,j \\ x_i \neq x_j}} a_{ij}) = -\frac{k}{2} + \sum_{\substack{i,j \\ x_i \neq x_j}} a_{ij}.$$

Therefore minimizing $Q(X)$ is equivalent to minimizing

$$\sum_{\substack{i,j \\ x_i \neq x_j}} a_{ij}.$$

This simply means we want to partition the

vertices of the graph G of interconnections into two sets (spins up and down or neurons on and off) in order to minimize the total weight $\sum a_{ij}$ of the edges joining the two subsets corresponding to the partition. This proves that the problem Min Cut [Garey,Johnson,1979] on a simple graph with weights $a_{ij} \in \mathbb{Z}^-$ is exactly equivalent to the problem of finding the ground state of the corresponding neural network with only inhibitory connections. The problem is known to remain NP hard if $a_{ij} = -1$ [Garey,Johnson,and Stockmeyer,1976] for any i and j (SIMPLE MIN CUT) and if in addition no vertex has degree exceeding 3. It can be solved in polynomial time if G is planar [Garey,Johnson,1979].

It should be noticed that the complexity of the optimization of a homogeneous quadratic form over H^n contrasts with the simplicity of its optimization over the n dimensional ball of radius R where the optimum is obtained on the surface of the sphere in the direction of an eigenvector corresponding to an extremal eigenvalue.

We shall now attempt to summarize several results relating the complexity of the optimization problem to the

structure of the graph G of interconnections and the nature of the thresholds and synaptic weights. When necessary we shall think to the form Q as an energy function:

$$Q(X) = -\frac{1}{2} \sum_{i,j} a_{ij} x_i x_j + \sum_i t_i x_i .$$

We have the theorem:

Theorem 8.2:

- (1) Min Q , Q in $\bar{F}_n^2(\mathbb{Z}^-)$ is in P .
- (2) Min Q , Q in $F_n^2(\alpha_{ij} \in \mathbb{Z}^+, t_i \in \mathbb{Z})$ is in P .
- (3) Min Q , Q in $\bar{F}_n^2(\mathbb{Z})$ where G is a tree is in P .
- (4) Min Q , Q in $F_n^2(\mathbb{Z})$ where G is a tree is in P .
- (5) Min Q , Q in $\bar{F}_n^2(\mathbb{Z})$ where G is planar is in P .
- (6) Min Q , Q in $\bar{F}_n^2(\mathbb{Z})$ where G is the 2-D quadratic lattice or the plane or the torus is in P .

Proof: (1) is trivial.

(2) see [Barahona,1985].

(3) left as an exercise.

(4) We have seen that the introduction in Q of a linear part or equivalently of non zero thresholds in the network can be seen as the addition of a new neuron interconnected to all the previous ones. This topological operation in general greatly increases the genus of G and as we shall see, is responsible for the transition $P \rightarrow NP$ for general planar graphs. Yet in the case of a tree it can be seen that this operation leaves the genus unchanged and equal to zero. Therefore (4) is a consequence of (5).

(5) see our discussion on MIN CUT above.

(6) see [Barahona,1982].

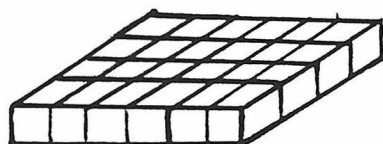
On the other hand, we have:

Theorem 8.3

- (1) Min Q , Q in $F_n^2(\alpha_{ij}=-1, t_i=1)$ and G is cubic planar is NP hard.
- (2) Min Q , Q in $\bar{F}_n^2(\{-1,0,1\})$ where G is a 2 levels grid is NP hard.
- (3) Min $\bar{F}_n^2(\{-1\})$ and every vertex of G has degree at most 3 is NP hard
- (4) Min $\bar{F}_n^2(\{-1,1\})$ where G is the hypercubic lattice and one dimension can be kept fixed (say to 4) is NP hard.

Proof: (1) see [Barahona,1982]. This point in particular shows the possible computational power of thresholds. In applications they can be stored locally and can introduce simplifications in the layout of the neural circuits. Real neurons are known to have non zero thresholds of the order of -70mv though there are additional reasons for this.

(2) see [Barahona,1982]. By 2 level grid we mean the graph:



(3) see our discussion on MIN CUT above.

(4) see [Bachas,1984].

Notice that in general the "clipping" of the synaptic strengths (i.e. $\alpha_{ij}=-1, 0$ or 1) does not really affect the complexity.

In dealing with NP complete problems planar circuits with 0-thresholds are not very well suited. Yet their ground

states and other properties can be computed in polynomial times. The ground state yields an optimal matching between frustrated faces [Barahona,1982]. Whether we could take advantage in real circuits of these computable characteristics, say for information storage, remains to be seen.

Reduction Algorithm

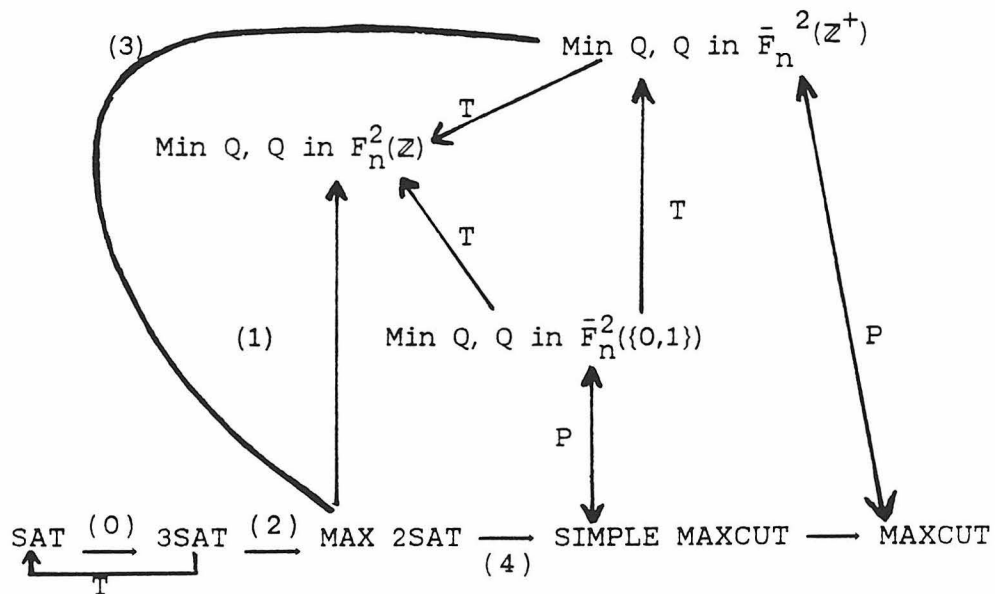
The results in the previous section indicate that any NP complete problem can be reduced to the optimization of a quadratic form even homogeneous with 0 and 1 coefficients over H^n . This encoding is particularly easy for some matching type situations. It is more difficult for boolean logic and moreover we have seen there exist problems that lead naturally to quartic energy networks. Logic gates cannot be represented directly by 0-threshold neurons with a quadratic energy function E . For these networks have a basic symmetry $E(-X) = E(X)$ which is violated by boolean functions. (If f is a boolean function in general it is not true that: $f(\bar{x}_1, \dots, \bar{x}_n) = f(x_1, \dots, x_n)$). Notice also that for applications, neural circuits where the synaptic connections strength are allowed to assume only two values, 0 or 1, are sometimes easier to implement. We shall therefore now investigate two types of questions:

- reduction of boolean logic to neural networks and vice versa.
- reduction of general networks to "clipped" networks with 0-1 connections.

We solve these problems here only for the most interesting case of quadratic energy functions, although the same type of techniques apply for $d > 2$. The results are obtained in a context of optimization, though there exist experimental

evidence [Hopfield,1982] also for the CAM applications. We shall use the notations of [Garey and Johnson,1979].

The key element in answering both questions is the introduction of an additional NP complete problem: MAX 2SAT. Given a set U of variables and a collection C of clauses over U , the satisfiability (SAT) problem consist in determining whether there is a satisfying truth assignment for C . If each c in C has $|c| = 3$ then the problem is called 3-satisfiability or 3SAT and both are NP complete. If for any c in C , $|c| = 2$ then the problem becomes solvable in polynomial time. Yet if we fix a positive integer K and ask if there exists a truth assignment for U that simultaneously satisfies at least K of the clauses in U ($K \leq C$), the task becomes NP complete and is called MAX 2SAT. MAX 2SAT enables the transformation of satisfiability problems into optimization problems. We shall explore the following table of reductions:



T = trivial P = refer to previous section (0) = see [Garey and Johnson,1979]

(1) Reduction of MAX 2SAT to Min Q, Q in $F_n^2(\mathbf{Z})$.

Keeping the same notation for literals in MAX 2SAT and variables of Q we can use the following encoding:

$$\begin{aligned} x_i &\longrightarrow x_i \\ \bar{x}_i &\longrightarrow 1 - x_i \quad (x_i \text{ are 0-1 variables}) \\ x_i \vee x_j &\longrightarrow x_i + x_j - x_i x_j . \end{aligned}$$

MAX 2SAT can then be converted into Max P, where P is obtained by adding all the quadratic forms corresponding to each clause in MAX 2SAT. Then $P(x_1, \dots, x_n) = K$ iff K clauses are satisfied by the corresponding assignment. Therefore MAX 2SAT is transformed into Min(-P) over the 0,1 hypercube. There exists a trivial one to one affine (and therefore polynomial) transformation from say the hypercube of a,b coordinates to the (1,-1) hypercube H^n . Therefore, the nature of the hypercube is irrelevant here. In conclusion MAX 2SAT can be simulated on a neural network with quadratic energy where the number of neurons is exactly equal to the number of literals in MAX 2SAT.

(2) Reduction of 3SAT to MAX 2SAT.

This is done in [Garey,Johnson,Stockmeyer,1976]. If 3SAT has $|C|$ clauses of 3 literals on m variables the corresponding MAX 2SAT has $7|C|$ clause on $m + |C|$ variables. Therefore, combining (1) and (2), 3SAT can be simulated on a neural network with $n = m + |C|$ neurons.

(3) Reduction of Min Q, Q in $F_n^2(\mathbf{Z}^+)$ to MAX 2SAT.

Let $Q = \sum \alpha_{ij} x_i x_j$ with $\alpha_{ij} \geq 0$, $x_i = \pm 1$. To each term of the form $\alpha_{ij} x_i x_j$ attach 2 α_{ij} clauses:

$$\alpha_{ij} \text{ times } \begin{array}{l} y_i \vee y_j \\ \bar{y}_i \vee \bar{y}_j \end{array} \quad \text{where } y_i = \frac{x_i + 1}{2} \quad i = 1, \dots, n .$$

Consider the corresponding MAX 2SAT on n boolean variables

with $2 \times \sum a_{ij}$ clauses. Notice that if $x_i \neq x_j$ then the 2 a_{ij} associated clauses are true, otherwise if $x_i = x_j$ only a_{ij} of these clauses are true. For a given assignment of the x_i and therefore y_i variables the number of clauses which are satisfied is given by:

$$\sum a_{ij}(y_i + y_j - y_i y_j) (1 - y_i + 1 - y_j - (1 - y_i)(1 - y_j)) =$$

$$\sum \left(\frac{3}{2} a_{ij} - \frac{1}{2} a_{ij} x_i x_j \right) = \frac{3}{2} \sum a_{ij} - \frac{1}{2} Q(x).$$

Therefore, minimizing Q is equivalent to maximizing the number of satisfied clauses.

These results partially solve the question of mapping SAT into neural networks and vice versa. We shall investigate now the reduction to "clipped" neural networks. By the general equivalence of NP complete problems, we know that such a reduction is possible. Since the capacity of quadratic forms on H^n is of the order of n^3 , and the capacity of clipped forms is at most of the order of n^2 we see that in order to be able to reduce any forms in $F_n^2(\mathbb{Z})$ to a form in $F_p^2(0,1)$, p must be at least of the order of $n^{3/2}$. But this is a lower bound and an explicit algorithm will yield an upperbound.

(4) Reduction of MAX 2SAT to SIMPLE MAX CUT.

This is done in [Garey, Johnson and Stockmeyer, 1976]. In particular it is shown that if MAX 2SAT has $|C|$ clauses on m variables one can construct a corresponding SIMPLE MAX CUT on a graph with $2(3|C|+1) + 2m + 2m(3|C|+1)$ vertices. In the same reference a careful description of the edges is of course also given. The equivalence of SIMPLE MAX CUT on a graph with n nodes and $\text{Min } Q, Q$ in $F_n^2(1,0)$ has already been seen. Hence, combining (3) and (4) we get:

Theorem 8.4:

Let $Q = \sum a_{ij} x_i x_j$ be a form in $F_n^2(\mathbb{Z}^+)$. Let $d = \sum a_{ij}$ and $m = \max a_{ij}$. Then the problem Min Q can be reduced to the problem Min P where P is in $F_p^2(0,1)$ and $p = (6d + 1)(2n + 2) + 2n$.

In particular we have: $p \leq O(mn^3)$.

Proof: Min Q can be transformed into MAX 2SAT with n literals and 2d clauses. MAX 2SAT can be reduced to a SIMPLE MAXCUT on a graph with p vertices, with:

$p = 2(6d + 1) + 2n + 2n(6d + 1)$. So: $p = (6d + 1)(2n + 2) + 2n$, and this last problem can be directly mapped into a clipped neural network containing p neurons. Since we have $d \leq \binom{n}{2} - n)m < \binom{n}{2} m$, we get $p \leq O(mn^3)$.

It would be interesting to have more knowledge about the properties of neural networks where m has a known fixed or variable upperbound. In [Minsky,Papert,1969] some "learning algorithms" where m grows exponentially are described. This is in contrast with the case for instance of the outerproduct formula with $d = 2$ on k vectors where a bound $m \leq k$ holds and k is certainly less than $O(n)$ in a context of CAM applications.

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Embeddings of Ultrametric Spaces in Finite Dimensional Structures

Abstract: Motivated by recent advances in theoretical physics and combinatorial optimization, we study the problem of embedding ultrametric spaces into finite dimensional structures: finite sets, euclidean spaces \mathbb{R}^n , euclidean sphere S^n , and n-dimensional hypercube with Hamming distance. We give conditions and constructions of embeddings and show a general upper bound of $n + 1$ on the cardinal of the ultrametric set. We also give an upper bound on the cardinal of quasi-ultrametric sets.

§1 Introduction

Definition 1.1: Let (X,d) be a metric space; that is X is a set and $d:X \times X \rightarrow \mathbb{R}^+$ is a distance function. The distance d is said to be ultrametric or non-archimedean if it satisfies:

$$d(x, z) \leq \max(d(x, y), d(y, z)) \quad (1)$$

Equivalently: every triangle is isocoles with the third side shorter or equal to the other two. The condition (1) implies immediately that for any two balls of radius R :

$$B(x, R) \cap B(y, R) \neq \emptyset \text{ implies } B(x, R) = B(y, R) \quad (2)$$

An important class of ultrametric spaces is obtained from non-archimedean valuations over fields. For instance the p-adic valuation $|\cdot|_p$ over the p-adic field \mathbb{Q}_p satisfies: $|x + y|_p \leq \max(|x|_p, |y|_p)$ and the corresponding distance: $d(x, y) = |x - y|_p$ is ultrametric.

Discrete ultrametric spaces are known to have a hierarchical tree-like organization and have been used for instance in taxonomy[4]. Recent advances in theoretical physics and combinatorial optimization seem to be based on the discovery of some underlying non-archimedean structure. In the replica symmetry breaking model for the Sherrington-Kirkpatrick spin glass the geometry of the

space of equilibrium states has been characterized by a hierarchic ultrametric structure [6]. A model for ultrametric information storage has been proposed in [8]. In [5] computer evidence is presented of an ultrametric organization of the 2-opt tours and the 3-opt tours in the travelling salesman problem. Similar ultrametric organization has been discussed in relation to graph coloring problems[3]. In all these cases bounds on the size of ultrametric structures can yield valuable information. In the case of the spin glass, a polynomial bound will have important consequences for the physical entropy. In the information storage models, capacity is crucial to practical applications and to biological modelling. In the optimization context, a polynomial bound on the number of λ -optima would be very surprising and might lead to algorithms yielding the shortest tour in polynomial time with probability 1. These applications are discussed in greater detail in [1].

We have thus been motivated to ask the following two questions: Let (E, d_e) and (X, d_x) be two metric spaces. Assume (X, d_x) is ultrametric. Then:

- (1) Can we embed X in E : ie can we find a subset Y of E isometric to (X, d_x) for the distance induced by d_e on Y , $(Y, d_e|_Y) \cong (X, d_x)$.
- (2) For a given E what is the maximal size of X for which such an embedding is possible?

We have studied these problems for the following metric spaces:

- a) Subsets of an n -elements set with the distance

$$d(X, Y) = \max(|X|, |Y|) - |X \cap Y| \quad (3)$$

- b) Hypercube of dimension n , ie n -dimensional vectors of coordinates $(0,1)$ or $(1,-1)$ with the Hamming distance d_h
- c) $E = \mathcal{R}^n$ with the euclidian distance.

In section 2 we prove preliminary results concerning a class of matrices. In sections 3 and 4 we prove the following basic theorem.

Theorem 1: For cases (a), (b), and (c), $|X| \leq n + 1$, and this bound is attained.

In section 5 we introduce trees. In section 6 we examine the general embedding problem. In section 7 we extend Theorem 1 to the case when almost every triangle satisfies equation 1. This extension is crucial to practical applications.

§2 A Class of Matrices

Given a finite family \mathcal{F} of real square matrices and $\lambda \in \mathfrak{R}$ with $\lambda \neq A_{ij}$ for all $A \in \mathcal{F}$, define $B = B(\mathcal{F}, \lambda)$ to be the square matrix with blocks $A \in \mathcal{F}$ on the main diagonal of B and each entry of B not in such a block equal to λ . The blocks $A \in \mathcal{F}$ will be termed the **maximal blocks** of $B(\mathcal{F}, \lambda)$. Evidently if $|\mathcal{F}| > 1 < |\mathcal{F}'|$ and $B(\mathcal{F}, \lambda) = B(\mathcal{F}', \lambda')$, then $\lambda = \lambda'$ and $\mathcal{F} = \mathcal{F}'$. That is the maximal blocks of $B(\mathcal{F}, \lambda)$ are uniquely determined, as is the parameter λ . Write $\mathcal{F}(B)$ and $\lambda(B)$ for these invariants.

Let \mathcal{B} be the intersection of all sets \mathcal{A} of square real matrices such that:

- (B1) Each 1 by 1 real matrix is in \mathcal{A} .
- (B2) If $\mathcal{F} \subseteq \mathcal{A}$ and $\lambda \in \mathfrak{R}$ with $\lambda \neq A_{ij}$ for all $A \in \mathcal{F}$ and all entries A_{ij} of A , then $B(\mathcal{F}, \lambda) \in \mathcal{A}$.

The matrices in \mathcal{B} will be termed **hierarchic**.

Define the **depth** of a 1 by 1 matrix to be 0, and, proceeding recursively, if $B \in \mathcal{B}$ with $|\mathcal{F}(B)| > 1$, define the depth $d(B)$ of B to be

$$d(B) = 1 + \max\{d(A) : A \in \mathcal{F}(B)\}.$$

Given $B \in \mathcal{B}$, define the set $\text{Blk}(B)$ of **blocks** of B as follows: If B is 1 by 1 then $\text{Blk}(B) = \{B\}$. If $d(B) > 0$ define

$$\text{Blk}(B) = \{B\} \cup \left(\bigcup_{A \in \mathcal{F}(B)} \text{Blk}(A) \right).$$

Partially order $\text{Blk}(B)$ by $A \leq C$ if $A \in \text{Blk}(C)$.

Define a matrix B to be **ultrametric** if B is hierarchic and $\lambda(A) < \lambda(C)$ for all $A, C \in \text{Blk}(B)$ with $A < C$. Define B to be **dual ultrametric** if $-B$ is ultrametric.

Lemma 2.1: Let B be a nonzero dual ultrametric matrix with all $B_{ij} \geq 0$. Then $\det(B) \neq 0$.

Proof: Recall that a real symmetric square matrix A is semidefinite positive if all eigenvalues of A are nonnegative reals and A is definite positive if all eigenvalues of A are positive reals. We use the following well known elementary fact:

(2.1.1) Let A, C be semidefinite positive and D definite positive. Then $A+C$ is semidefinite positive and $A+D$ is definite positive.

Let $\lambda = \lambda(B)$ and n the size of B . Let J be the n by n matrix all of whose entries are 1. Then $B = \lambda J + A$, where A is a dual ultrametric matrix with $\lambda(A)=0$ and $0 \neq A \geq 0$. Observe λJ is semidefinite positive. Moreover if B is of depth 0, then as $B \neq 0$, $B = \lambda J = \lambda$ is definite positive. Hence, proceeding by induction on the depth of B , B is the sum of semidefinite positive matrices with a definite positive diagonal matrix. We conclude from (2.1.1) that B is definite positive. In particular $\det(B) \neq 0$.

Lemma 2.2: Let B be a nonzero hierarchic matrix of size N . Then

- (1) The rank of B is at least $\frac{N}{2}$.
- (2) If $N \geq 4$ and $\lambda(B) \neq 0$, then B has rank at least $\frac{N}{2} + 1$.

Proof: We perform certain row and column operations on B . Let $\mathcal{F}(B) = (B(1), \dots, B(n))$ and let N_k be the size of $B(k)$. Set $m = N_1$. Let 1B be the matrix obtained by subtracting the first row of B from all other rows. Observe ${}^1B(k)$ remains hierarchic and $\lambda({}^1B(k)) \neq 0$ for $k > 1$. Hence by induction on N ,

$$(2.2.1) \text{rank}({}^1B(k)) \geq \frac{N_k}{2} + 1 \text{ if } N_k \geq 4.$$

It is easy to see that

$$(2.2.2) \text{rank}({}^1B(k)) \geq 1, 1, 2 \text{ for } N_k = 1, 2, 3, \text{ respectively. In particular in this case } \text{rank}({}^1B(k)) \geq \frac{N_k}{2}.$$

Similarly 2.2.1 and 2.2.2 hold if $k=1$. Next subtract the first row of ${}^1B(k)$ from the remaining rows of ${}^1B(k)$, for each $k > 1$. Denote the resulting matrix by 2B . Define m to be the size of the block $B(1)$ and write 2D_i for the row vector $({}^2B_{i1}, \dots, {}^2B_{im})$ of 2B . Let $v = B(1)_1$ be the first row of $B(1)$ and $\lambda(m)$ the row vector of length m all of whose entries are λ . Observe that ${}^2D_i = 0$ if $i > m$ and i is not the first row of some block, while ${}^2D_i = \lambda(m) - v$ whenever i is the first row of a block ${}^2B(k)$ with $k > 1$. Observe also that the entry in the upper right hand corner of ${}^2B(k)$ is $\lambda(B(k)) - \lambda = \sigma_k \neq 0$. Thus if $N_k = 1$,

§3 Ultrametricity

Recall that an **ultrametric space** is a pair (S,d) where S is a nonempty set and d is a non-archimedian distance function on S . Define a function $d:S \times S \rightarrow \mathfrak{R}$ to be **dual-ultrametric** if and only if for all $r, s, t \in S$, $d(s, s) > d(s, r) \geq \min\{d(s, t), d(r, t)\} \geq 0$. Finally define $d:S \times S \rightarrow \mathfrak{R}$ to be **trimetric** if d -diag(d) is ultrametric and $d(x,x) \neq d(x,y)$ for all distinct $x, y \in S$, where $\text{diag}(d)=d(x,y)$ if $y=x$ and 0 otherwise.

Let (S,d) be an ultrametric or trimetric space and define

$$\lambda(S) = \max\{d(a,b) : a, b \in S \text{ and } a \neq b\}.$$

For $a \in S$ define

$$\Delta(a) = \{s \in S : d(a,s) < \lambda(S) \text{ or } s = a\}.$$

Call $\Delta(a)$ the **neighborhood** of a .

Lemma 3.1: The set $\{\Delta(a) : a \in S\}$ of neighborhoods is a partition of S such that $\Delta(a) = \Delta(b)$ for all $b \in \Delta(a)$.

Proof: Let $a \in S$ and suppose $b \in S - \Delta(a)$. Let $c \in \Delta(a)$. Claim $\Delta(a) = \Delta(c)$. We may suppose $c \neq a$. Then $d(a,b) = \lambda > d(a,c)$, so as S is ultrametric, $d(b,c) = \lambda$. Hence $S - \Delta(a) \subseteq S - \Delta(c)$. By symmetry, $S - \Delta(a) = S - \Delta(c)$, so indeed $\Delta(a) = \Delta(c)$.

Next if $s \in S$ then either $s \in \Delta(a)$ or $s \in S - \Delta(a)$. In the first case $S - \Delta(s) = S - \Delta(a)$ is nonempty by paragraph one. In the second, $a \in S - \Delta(s)$, which is then nonempty. So in any event $S \neq \Delta(s)$. Hence by paragraph one, $\Delta(s) = \Delta(t)$ for each $t \in \Delta(s)$. Thus the lemma is established.

Define the **depth** $\text{dep}(S)$ of (S,d) recursively as follows: If $|S| = 1$ let $\text{dep}(S)=0$. Otherwise $\text{dep}(S) = 1 + \max\{\text{dep}(\Delta(a)) : a \in S\}$.

Let $(S_i : 1 \leq i \leq m)$ be the set of neighborhoods $\Delta(a)$, $a \in S$, as in (3.1). Order S so that the members of S_i proceed those of S_j for $i < j$, and proceeding recursively, so that each S_i and its subneighborhoods are ordered subject to the same constraint. The **distance matrix** of (S,d) is the square matrix $B=B(S)$

whose rows and columns are indexed by S and with $B_{st} = d(s, t)$ for each $s, t \in S$. Observe

Lemma 3.2: If (S, d) is trimetric or ultrametric then its distance matrix $B(S)$ is a hierarchic matrix with $\lambda(S) = \lambda(B(S))$. If (S, d) is dual ultrametric then $B(S)$ is a dual ultrametric matrix.

Proof: This is immediate from (3.1) and the ordering of S .

Lemma 3.3: Let V be the space of n -tuples with 0,1 entries, and d the standard inner product on V ; that is $d(u, v)$ is the number of common nonzero entries in $u, v \in V$. Let $n > 1$ and $S \subseteq V$.

- (1) If (S, d) is trimetric then $|S| \leq 2(n - 1)$.
- (2) If (S, d) is dual ultrametric then $|S| \leq n$.

Proof: Let $N = |S|$ and A the N by n matrix whose row vectors are the vectors in S . Observe that if A^T denotes the transpose of A , then $AA^T = B(S)$.

Embed V in n -dimensional Euclidean space \mathfrak{R}^n and regard A^T as a linear map from \mathfrak{R}^n into \mathfrak{R}^N . Then the subspace U of \mathfrak{R}^N generated by S has dimension at least $\dim(UA^T) = \text{rank}(B(S))$. So $n \geq \text{rank}(B(S))$. Hence lemmas 2.1 and 2.2 complete the proof.

Lemma 3.4: Let S be a set of nonempty subsets of a finite set X of order $n > 1$. For $s, t \in S$, let $d(s, t) = |s \cap t|$. Then

- (1) If (S, d) is trimetric then $|S| \leq 2(n - 1)$.
- (2) If (S, d) is dual ultrametric then $|S| \leq n$.

Proof: This is equivalent to 3.3 since V is isometric with the set of all subsets of X via the map which takes a vector in V to its support.

Notice that the upper bounds in 3.3 and 3.4 are attained. In 3.4.2 take S to be the set of subsets of X of order 1. In 3.4.1 let X be the set of vectors in an m -dimensional vector space W over the field of order 2 and let S be the set of cosets of all hyperplanes of W . Then $n = 2^m$ and $|S| = 2(2^m - 1)$. In this latter example S is of depth 2 with distances 2^{m-1} , 2^{m-2} , and 0.

Lemma 3.4.2 follows from a result of Ryser[9] when the depth of S is 1.

we can add suitable multiples of column i through ${}^2B(k)$ to the first m columns of 2B to insure that ${}^3D_i = 0$, where 3B is the image of 2B under these column operations.

In particular suppose that 3B_i , $i \in I$ is a set of row vectors of 3B and $\sum_{i \in I} a_i ({}^3B_i) = 0$ is a linear dependence. Let $I(k)$ consist of those indices in I indexing rows in $B(k)$. Assume for each k with $N_k > 1$, the first row r_k of $B(k)$ is not in I . Then from the structure of 3B , $\sum_{i \in I(k)} a_i ({}^3B_i) = 0$ for each k . Order the rows of $B(k)$ so that the last $N_k - 1$ rows contain a basis of the row space of ${}^1B(k)$ if ${}^1B(k)$ is singular. Thus

(2.2.3) $\text{rank}(B) \geq (\sum_k \text{rank}({}^1B(k))) - \epsilon$, where ϵ is the number of k such that $N_k > 1$ and ${}^1B(k)$ is nonsingular.

Assume $N \geq 4$. We conclude from 2.2.1 through 2.2.3 that $\text{rank}(B) \geq \frac{N}{2}$ and either $\text{rank}(B) \geq \frac{N}{2} + 1$ or $N_k = 2$ and $\text{rank}({}^3B(k)) = 1$ for all but at most one k_0 for which $N_{k_0} = 1$ or 3. Of course we may assume the latter and choose our ordering so that $R = ({}^3B_i : i \in I)$ is linearly independent of order M with $M \geq \frac{N}{2}$, $N_j = 2$ for some $1 < j$, and with 1 not in I . To complete the proof, we may assume $\lambda(B) = \lambda \neq 0$, and it remains to show 3B_1 is independent of R . Let π be the projection of the row space on its last $N-m$ coordinates. Then 3B_1 has all entries λ and is in the space spanned by $I\pi$. This is not the case as the projection of ${}^3B(j)$ on the two columns through $B(j)$ does not contain (λ, λ) since $\text{rank}({}^3B(j)) = 1$.

Indeed our proof was suggested by Ryser's.

Lemma 3.5: Let V be the space of n -tuples with 0,1 entries and d the Hamming metric on V ; that is $d(u,v)$ is the number of nonzero entries in u and v not common to u and v . Then $|S| \leq n + 1$ for each ultrametric subset (S,d) of V .

Proof: This is a special case of 4.1 in the next section, but the proof in this special case is a little easier, and thus perhaps worth giving.

Let $N = |S|$ and let A be the N by n matrix whose rows are indexed by S and with $A_{sj} = 1$ or -1 when $s \in S$ has 1 or 0 as its j th entry. Observe $AA^T = 2D - nJ$, where J is the N by N matrix with all its entries 1 and $D = nJ - B(S)$. Moreover D is dual ultrametric with $D \geq 0$. Now arguing as in 3.3, the subspace U of \mathfrak{R}^n generated by S has dimension at least $\text{rank}(D) - 1$, as its image in \mathfrak{R}^N is spanned by the translates of the row vectors of $2D$ by the vector (n, \dots, n) . Hence Lemma 2.1 completes the proof.

§4 Euclidean Space

In this section V is n -dimensional Euclidean space over \mathfrak{R} . For $u, v \in V$ let $\langle u, v \rangle = |u - v|$. We prove:

Lemma 4.1: Let S be an ultrametric subspace of V . Then $|S| \leq n + 1$. Indeed translating to get $0 \in S$, $S - \{0\}$ is linearly independent.

Assume S is an ultrametric subset of V of order N . Let $\lambda = \lambda(S)$. For $s \in S$, define $S(s) = S - \Delta(s)$. Thus $S(s)$ is the set of points in S on the sphere of distance λ from s , and $\Delta(s)$ is the set of points of S in the interior of that sphere.

As translation preserves the collection of ultrametric subsets of V , we may indeed take $0 \in S$. We first prove:

Lemma 4.2: $S(0)$ is linearly independent.

Proof: Let A be the matrix of row vectors of $S(0)$. Then $AA^T = \lambda J - \frac{B(S(0))}{2}$. Notice AA^T is dual ultrametric. This is because $B(S(0))$ is ultrametric and

each entry on the main diagonal of AA^T is greater than each entry off the main diagonal. Indeed each entry on the main diagonal is λ while entries off the main diagonal are of the form $\langle s, t \rangle < \lambda$ as $s \neq t$ and $|s| = |t| = \lambda$.

As AA^T is dual ultrametric, $\text{rank}(AA^T) = N$ by 2.1. Thus A^T is a surjective map from the subspace of V spanned by $S(0)$ onto \mathfrak{R}^N so as that space is of dimension $d \leq N$, it follows that $d = N$ and $S(0)$ is linearly independent. So Lemma 4.2 is established.

Lemma 4.3: $\Delta(0) - \{0\}$ is linearly independent.

Proof: Let $a \in S(0)$. Then $\Delta(0) \subseteq S(a)$, so $\{s - a : s \in \Delta(0)\}$ is linearly independent by 4.2. Hence $\Delta(a)$ has a linearly independent subset of order $|\Delta(a)| - 1$, so as $0 \in \Delta(0)$ the lemma follows.

Let $\Delta(0) = \{x_0, \dots, x_m\}$ with $x_k = (x_{k1}, \dots, x_{kn})$ and $x_0 = 0$. Appealing to 4.3 and replacing S by an image under some suitable orthogonal transformation of \mathfrak{R}^n , we may assume $x_{kj} = 0$ for $j > k$ and $x_{kk} = e_k \neq 0$. Let π_k be the projection of V onto the subspace V_k of V consisting of those vectors with 0 in the first k coordinates.

Lemma 4.4: (1) There exist $r_i \in \mathfrak{R}, 1 \leq i \leq m$, such that for all $s = (s_1, \dots, s_n) \in S(0)$, $s_i = r_i$.

(2) $S(0)\pi_m$ is a linearly independent subset of V_m .

Proof: We prove the analagous statements for $k \leq m$ by induction on k . For $k=0$ this is 4.1. Assume the result for $k-1$. Then for $s \in S(0)$, $\lambda = |s| = \sum s_i^2 = |s - x_k| = \sum (s_i - x_{ki})^2$. So $0 = \sum (x_{ki}^2 - 2x_{ki}s_i) = D - 2e_k s_k$, where $D = e_k^2 + \sum_{i < k} (x_{ki}^2 - 2x_{ki}r_i)$. Thus (1) holds for k with $r_k = \frac{D}{2e_k}$. Moreover $|s\pi_k| = \lambda - \sum_{i \leq k} r_i^2 = \lambda_k$, and for $s \neq t \in S(0)$, $|s\pi_k - t\pi_k| = |s - t|$, so $S(0)\pi_k$ is on the sphere of distance λ_k from 0 in V_k and $S(0)\pi_k$ is ultrametric in V_k . Therefore (2) holds by 4.1.

Notice that 4.4 completes the proof of Lemma 4.1 and that Lemmas 3.4, 3.5, and 4.1 complete the proof of Theorem 1 in cases a, b, and c respectively. Also as a simple consequence we have the following:

Theorem 4.5: The maximal ultrametric set that can be embedded in the euclidian sphere S^n has cardinal $n+2$.

Proof: The sphere S^n is trivially embedded in the euclidian space \mathbb{R}^{n+1} . Therefore an upper bound of $n + 2$ holds. On the other hand the $n+1$ -dimensional hypercube can be embedded in S^n with the euclidian distance via some trivial scaling. Ultrametric sets on the hypercube with Hamming distance are still ultrametric in \mathbb{R}^n with Euclidean distance. Therefore the value $n+2$ is attained.

§5 Trees

We shall first consider the tree representation for ultrametric spaces. Let $T=(V,E)$ be a rooted tree with vertices V , edges E , and root α , $\alpha \in V$. We will define the leaves of T to be the monovalent vertices other than the root. Let $X = \{x_1, \dots, x_k\}$ be the set of leaves of T . Let $w:E \rightarrow \mathbb{R}^+$ be a weight function defining the length of each edge. Let d_T be the corresponding metric on the tree. Assume that:

$$\text{There exists } h > 0 \text{ such that } d_T(\alpha, x_j) = h \text{ for all } j, 1 \leq j \leq k. \quad (5.1)$$

h is called the height of the tree. More generally for every vertex v define the height $h(v)$ of v to be the length of a minimal path which connects v to a leaf. Because of 5.1, $h(v)$ is well defined.

Define a metric space (X, d_X) by letting the distance between two leaves be the height of their first predecessor. Again 5.1 renders d_X well defined. It is easy to check that (X, d_X) is an ultrametric space. Moreover it can easily be shown by arguments like those of section 2 that every finite ultrametric space can be represented by such a tree.

The leaves can be partitioned into l sets: B_1, \dots, B_l of nearest neighbours. We shall denote by b_i the cardinal of B_i and d_i the common distance of the leaves in B_i to their first predecessor. From now on any finite ultrametric space (X, d_x) will be an ultrametric tree with the previous conventions and with an ultrametric positive 0-diagonal distance matrix D .

We need to derive a few general matrix equations. Cases (a) and (b) with the (1,-1) conventions yield the most simple expressions and this will suffice.

CASE (a): Let Y_1, \dots, Y_k be subsets of an n -elements set with distance:

$$d(Y_i, Y_j) = \max(|Y_i|, |Y_j|) - |Y_i \cap Y_j|$$

Let A be the $k \times n$ incidence matrix and M be the $k \times k$ matrix defined by:

$$m_{ij} = \max(|Y_i|, |Y_j|)$$

Then:

$$AA^t = M - D \tag{5.2}$$

In the special case where all the subsets have the same cardinality v , (5.2) yields

$$AA^t = vJ - D \tag{5.3}$$

CASE (b): Let X_1, \dots, X_k be k n -dimensional vectors of coordinates (1,-1) with the Hamming distance d_h . Let B be the matrix having X_i as its i -th row. Then:

$$BB^t = nJ - 2D \tag{5.4}$$

In these cases our two initial questions become: If D is a positive 0-diagonal ultrametric matrix under which conditions can we solve equations (5.2) and (5.4)? What is the maximal value for k if n is fixed? Notice that the tree for which the upper bound $n+1$ of section 3 is attained has a very poor structure. One might wonder if much tighter upper bounds could be obtained for classes of trees with a richer branching structure. We shall prove now that this not the case and examine the general embedding problem: given a fixed ultrametric tree T can we embed it in one of the metric spaces of type (a) (b) or (c) ?

§6 General Embeddings

We first discuss case (a).

Theorem 6.1: Let T be an ultrametric tree with k leaves and D be the corresponding k by k matrix of distances. Assume D has integer entries. Then we can

always embed T in an n -set for n large enough. More precisely: we can find an n -set and k of its subsets with fixed cardinal v such that the equation: $vJ - D = AA^t$ is satisfied. Moreover if h denotes the height of the tree, then $v = h$ and

$$n = h + \sum_{i=1}^l (b_i - 1)d_i + \sum_{i=1}^{l-1} d_{ii+1},$$

where $d_{ii+1} = d(x_i, x_j)$ for $x_i \in B_i$ and $x_j \in B_{i+1}$.

Proof: Trivially it is necessary for the distance matrix D of T to have integer coefficients and since the weights are differences of distances they too are integers. Suppose now we are given a tree of height h such that all the weights $w(e)$ are integers. We shall construct recursively the n -set and its k h -element subsets by assigning to each vertex v of T a certain subset $f(v)$.

Let (a_n) be a list of variables. Let $P_1 \dots P_k$ be any ordering of the k unique directed paths joining the root α to the leaves x_i , $1 \leq i \leq k$. Order the vertices of T lexicographically considering first the ordering of the paths and then the order within each path.

step 1: $f(v_1) = f(\alpha) = \emptyset$

step m : Assume that $f(v_i)$ has been defined for $i \leq m$ so that $f(v_i) \subseteq f(v_j)$ if $i \leq j$ and v_i and v_j are on a common path. Let $\bigcup_{i=1}^{m-1} f(v_i) = \{a_0, a_1, \dots, a_{g(m)}\}$. There exists a unique $p < m$ with v_p joined to v_m . Let w denote the weight of the corresponding edge. Then we set:

$$f(v_m) = f(v_p) \cup a_{g(m)+1}, \dots, a_{g(m)+w}.$$

For any leaf x_i we have: $|f(x_i)| = h$ since we start with $f(\alpha) = \emptyset$ and we add $w(e)$ new elements for any edge e belonging to the directed path between α and x_i . Let $Y_i = f(x_i)$ $i = 1, \dots, k$. Then by construction:

$$\max(|Y_i|, |Y_j|) - |Y_i \cap Y_j| = d(x_i, x_j)$$

which is the height of the common predecessor of x_i and x_j . Therefore Y_1, \dots, Y_k are k h -elements subsets of an n -set: $\bigcup_{i=1}^k f(x_i) = \bigcup_{v \in V} f(v)$ representing the given ultrametric tree T . Moreover by construction: $|\bigcup_{x \in B_i} f(x)| = h + (b_i - 1)d_i$. Therefore deleting all but one leaf from each block and proceeding by induction on k , we get:

$$n = h + \sum_{i=1}^l (b_i - 1)d_i + \sum_{i=1}^{l-1} d_{ii+1}$$

We next consider case (b).

We are given an ultrametric tree T and we are looking for an embedding into some n -dimensional hypercube. As in case (a) it is easy to see that all the weights need to be integers. The same holds for h . But additional conditions are necessary as shown by the following simple lemma:

Lemma 6.2: Every triangle on the hypercube with Hamming distance d_h has an even perimeter.

As a consequence, for every ultrametric isocoles triangle on the hypercube the third side cannot have odd length. It is easy to show by induction that a necessary condition for the existence of an embedding is that the tree T has one of the following two exclusive properties:

- (i) All the weights are even integers.
- (ii) The root α has only two adjacent vertices v_1 and v_2 , $w(\alpha, v_1)$ and $w(\alpha, v_2)$ are odd, and all the other edges have even weights.

Such a tree will be called **hypercubic**. We can now state the following:

Theorem 6.3: Let T be an ultrametric hypercubic tree with k leaves and distance matrix D . Then we can always embed T in an n -dimensional hypercube for n sufficiently large. More precisely: we can find k n -dimensional vectors X_1, \dots, X_k of coordinates $(1, -1)$ such that the equation $BB^T = nJ - 2D$ is satisfied. Moreover

if all edges have even length we can choose the k vectors in one of the hyperplanes:

$$\sum_{i=1}^n x_i = c = \pm(n - h)$$

if the first two edges e_1 and e_2 have odd lengths $2a + 1$ and $2b + 1$ then we can choose the vectors corresponding to e_1 to be in one of the hyperplanes:

$$\sum_{i=1}^n x_i = \pm(n - 2c_1)$$

and those corresponding to e_2 in one of the hyperplanes:

$$\sum_{i=1}^n x_i = \pm(n - 2c_2)$$

with the same sign in both equations, where c_1, c_2 are two integers satisfying:

$$c_1 + c_2 = h$$

and

$$c_1 \geq \frac{(h - 2a - 1)}{2}$$

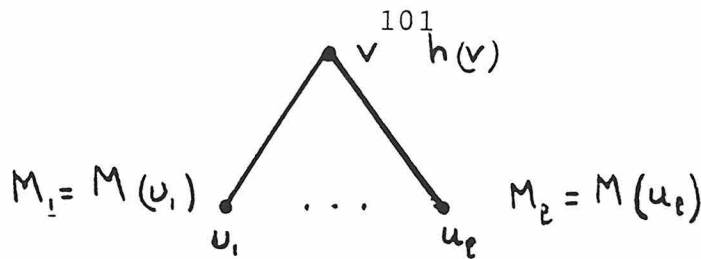
and

$$c_2 \geq \frac{(h - 2b - 1)}{2}.$$

Proof: For convenience we shall use $(0,1)$ coordinates rather than $(1,-1)$. The **weight** of a vector will be the cardinal of its non zero coordinates. If all row vectors in a matrix M have same weight w , we shall write $w(M) = w$: the weight of the matrix M . Proceeding recursively by height we shall now construct our embedding by attaching progressively to each vertex v of the tree a matrix $M(v)$ of weight $\frac{h(v)}{2}$. (except for the leaves x_i where $w(M(x_i)) = 1$). Notice that we assume that all edges except perhaps the last two have even length. The matrix $M(\alpha)$ will provide the final embedding. The number of rows of $M(v)$ will be equal to the number of leaves attached to v .

We start by defining $M(x_i) = 1$ for every leaf x_i . Obviously $w(M(x_i)) = 1$. Suppose we are looking now at a vertex v to which no matrix has been assigned. If $\{u_1, \dots, u_l\} = \{u \in V : h(u) \leq h(v) \text{ and } (u, v) \in E\}$ and if $M(u_i)$ has been defined for $1 \leq i \leq l$ then we shall define a matrix $M(v)$ for the vertex v through a process called amalgamation. We shall denote: $M(v) = [M(u_1), \dots, M(u_l)]$. We then iterate amalgamation as many times as necessary until $M(\alpha)$ is obtained. The rows of $M(\alpha)$ will represent the final vectors on the hypercube.

Definition of amalgamation: Assume we have the following situation:



Assume that M_i is $n_i \times m_i$ and $w(M_i) = \frac{h_i}{2}$ $i = 1, \dots, l$ and that n_i is the number of leaves attached to u_i . Since $h_i \leq h(v)$ we can define an integer λ_i by: $\frac{h_i}{2} + \lambda_i = \frac{h(v)}{2}$ for $i = 1, \dots, l$. Then define $M = [M_1, \dots, M_l]$ by:

$$M = \begin{pmatrix} J_1 & 0 & & 0 & M_1 & 0 & & 0 \\ 0 & J_2 & & 0 & 0 & M_2 & & 0 \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ 0 & 0 & & J_l & 0 & 0 & & M_l \end{pmatrix}$$

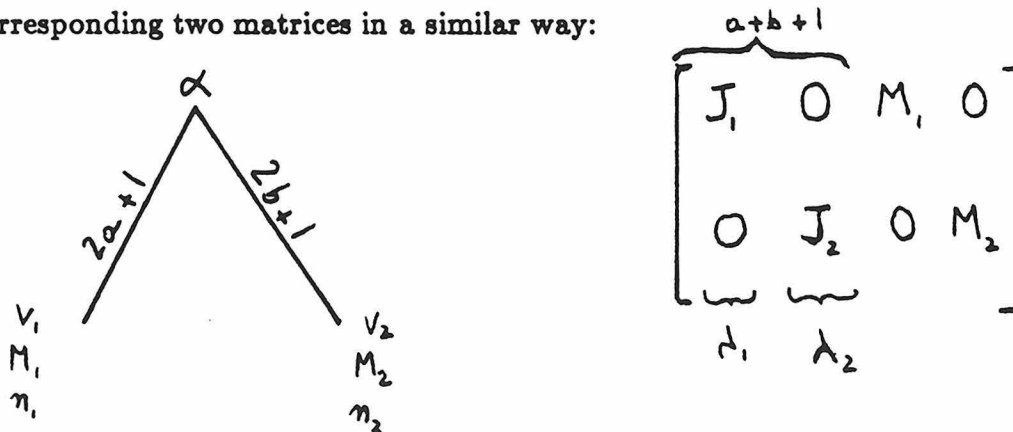
where J_i is the $n_i \times \lambda_i$ matrix all of whose entries are 1. M has the following properties:

- (1) $w(M) = w(M_i) + \lambda_i = \frac{h_i}{2} + \frac{h(v)}{2} - \frac{h_i}{2} = \frac{h(v)}{2}$
- (2) M is $n \times m$ where $n = \sum_1^l n_i$ and $m = \sum_1^l (m_i + \lambda_i)$ and n is the number of leaves attached to v .
- (3) the Hamming distance between any two rows i and j of M belonging to two different blocks is given by:

$$d_{ij} = w(M_i) + \lambda_i + w(M_j) + \lambda_j = h(v)$$

which is exactly the ultrametric distance between the corresponding two leaves.

If the last two edges have odd length we define the amalgamation for the corresponding two matrices in a similar way:



$\lambda_1 + \lambda_2 = a + b + 1$ and $h_1 + 2a + 1 = h_2 + 2b + 1$. If all edges are even we have from (1): $w(M(\alpha)) = \frac{h}{2}$. Therefore if we are using a (1,-1) representation

the vectors lie in the hyperplane:

$$\sum_{i=1}^n x_i = \frac{h}{2} - (n - \frac{h}{2}) = h - n$$

or its mirror image. If the last two edges e_1, e_2 have odd lengths then the vectors are separated into two groups of constant weight: $w_1 = \frac{h_1}{2} + \lambda_1$ and $w_2 = \frac{h_2}{2} + \lambda_2$. Since $\lambda_1 + \lambda_2 = a + b + 1$ we have $w_1 + w_2 = h$ and:

$$w_1 \geq \frac{h - 2a - 1}{2}, w_2 \geq \frac{h - 2b - 1}{2}.$$

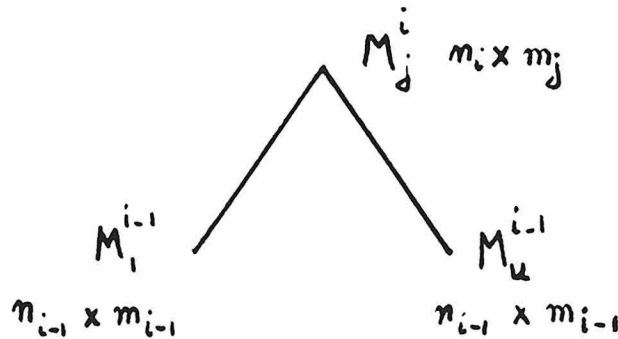
Finally using (1),(2) and (3) it is easy to show that the matrix $M(\alpha)$ yields the required embeddings.

Let us now consider regular trees and compute the corresponding dimension n of the hypercube.

Theorem 6.4: Let T be a tree such that every vertex with the exceptions of the leaves has a fixed number of successors u . Assume that all edges have a constant even length $2l$. Let $h=2ml$. Then T can be embedded in an n -dimensional hypercube with:

$$n = ul \left(\frac{u^m - 1}{u - 1} \right)$$

Proof: Consider the amalgamation step:



We have $n_i = un_{i-1} + ul$ and $n_1 = ul$. Therefore solving this recurrence relation, we get:

$$n = \sum_{i=1}^m lu^i = ul \left(\frac{u^m - 1}{u - 1} \right)$$

Corollary 6.5: Let n be fixed. Then we can embed in the hypercube H_n an ultrametric tree with constant even valence u (with the exception of the leaves)

and edges of constant even length $2l$ corresponding to an ultrametric set of size at least k :

$$k \geq \frac{(n+1)(u-1)}{u^{2l}} + \frac{1}{u}$$

Proof: If $n = ul \frac{u^m - 1}{k - 1}$ then the size is $k = u^m$. Therefore the worst case corresponds to: $n = ul \left(\frac{k^{m+1} - 1}{k - 1} \right) - 1$ for which the size is still $k = u^m$. Solving for k we get the bound of the theorem. Asymptotically this indicates that hypercubic trees with a rich branching structure can be embedded into the hypercube, the bound on the size being still of the form $O(n)$.

Finally we consider case (c)

We are now given a tree T and want to embed it in \mathbb{R}^n . Surprisingly enough it is not true that every finite metric space can be embedded in \mathbb{R}^n for n large enough and with the euclidian distance.

One obvious reason for that is that for any three points not on a same line the triangle inequality need to be strict. Yet this does not yield a sufficient condition of embeddability since counterexamples can be found by slightly perturbing cases where the triangle inequality is not strict.

If the finite metric space is ultrametric then the triangle inequality is obviously strict for any three distinct points.

We can now prove the following:

Theorem 6.6: Every finite ultrametric space with rational matrix distance D can be embedded into the euclidian space \mathbb{R}^n , for n large enough. Moreover the points can be chosen in one of the hyperplanes of equation

$$\sum_{i=1}^n x_i = \pm(n - h)$$

Proof: The idea is to use scaling on the given distances, obtain a new set that can be embedded into an hypercube and then go back to \mathbb{R}^n . Since D is assumed to have rational entries we can find a constant c such that the matrix cD has integers entries which are also multiples of 4. Construct a new matrix D' with entries $d'_{i,j}$ defined by:

$$d'_{i,j} = \frac{c^2 d_{i,j}^2}{4}$$

Notice that by construction $d'_{i,j}$ is even. Moreover it is easy to check that the matrix D' defines an ultrametric space. Therefore using Theorem 6.2 the corresponding set can be embedded into an n -dimensional hypercube with Hamming distance for n large enough. For points on the hypercube with $1, -1$ coordinates the Hamming distance and the euclidian distance are related by: $d_e = 2\sqrt{d_h}$. Therefore the previous construction yields in fact an embedding in \mathbb{R}^n with distance matrix cD . To obtain the final embedding we now only need to rescale by a factor of $\frac{1}{c}$. Because of theorem 6.3 the points can be chosen in one of the hyperplanes:

$$\sum_{i=1}^n x_i = \pm(n - h)$$

We can now extend this to show that every ultrametric space with $n + 1$ or fewer points can be embedded in \mathbb{R}^n .

Theorem 6.7: Let X be a finite ultrametric space of cardinal m with real distance matrix D . Then X can be embedded into \mathbb{R}^{m-1} .

Proof: Let us denote by $D(x_1, \dots, x_k)$ the bordered symmetric determinant of order $k+1$:

$$\begin{vmatrix} 0 & 1 & 1 & \dots & 1 \\ 1 & 0 & (d_{12})^2 & \dots & (d_{1k})^2 \\ 1 & (d_{12})^2 & 0 & \dots & (d_{2k})^2 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & (d_{1k})^2 & (d_{2k})^2 & \dots & 0 \end{vmatrix}$$

The following theorem by Menger can be found in [2]:

A necessary and sufficient condition that a semimetric space X may be congruently embedded in the euclidean n -dimensional space \mathbb{R}^n is:

- (1) For each positive integer k , $2 \leq k \leq n + 1$, and each set of k points x_1, \dots, x_k of X , $\text{sgn } D(x_1, \dots, x_k) = (-1)^k$ or 0 .
- (2) Each set of $n+2$ points of X has a vanishing bordered symmetric determinant.

Recall that if d is ultrametric so is d^2 . Also note that if $n = m - 1$, condition (2) is trivially satisfied.

Assume now for contradiction that we can find k points x_1, \dots, x_k of X violating condition (1). The corresponding bordered determinant therefore has sign

$(-1)^{k+1}$. Yet we can slightly perturb the ultrametric matrix of distances between the points x_1, \dots, x_k so that the newly obtained matrix is still ultrametric and has rational entries. Therefore, by Theorem 6.6 and Menger's result the corresponding bordered determinant can not have sign $(-1)^{k+1}$. Since the rational approximation of the d_{ij} and hence of the d_{ij}^2 can be made with arbitrary precision, a contradiction arises by continuity.

§7 Quasi-Ultrametric Structures

For practical applications one must study structures that are quasi ultrametric in some sense. There are two natural cases: first where every triangle violates the ultrametric constraint by only a small amount; and second where almost every triangle satisfies the constraint exactly, but a small subset is allowed to violate ultrametricity. We introduce two definitions and state corresponding results.

Definition 7.1: Let (E,d) be a metric space and X a subset with the induced metric. (X,d) is ϵ -ultrametric if and only if there exists an ultrametric subspace (Y,d) of (E,d) such that: for all $x_1, x_2, x_3 \in X$, there exists $y_1, y_2, y_3 \in Y$ with $y_i \in B(x_i, \epsilon)$.

In reference[8], \sqrt{n} -ultrametric structures on the hypercube are considered. Using Stirling's formula it is easy to see that $|B(x, \sqrt{n})|$ is exponential and therefore \sqrt{n} -ultrametric structures may be exponential in size. The same should hold for any $f(n)$ -ultrametric structure on the hypercube where $f(n)$ is an increasing unbounded function of n .

In many of the applications, one considers a sequence $((X_n, d), Y_n)$, where the (X_n, d) are metric spaces and the Y_n are finite subspaces which have the property that in the limit as $n \rightarrow \infty$, almost every triangle in Y_n satisfies the ultrametric condition 1.1 under the induced metric. For example, in the case of infinite range spin glasses, (X_n, d) is \mathfrak{R}^n under the euclidean metric and Y_n is a set of n -vectors, the "thermodynamic equilibrium states". Describing the set Y_n is fundamental to understanding the physics of the model. It has been shown, in the "R.S.B." model (a model believed to accurately reflect the physics),

that in the limit of large n , the probability that any triangle among the Y_n will satisfy the ultrametric constraint is one [6]. An important question is whether one can bound $k_n = |Y_n|$ by some polynomial in n . Such a bound will follow from Theorem 1 (for the cases (a),(b), and (c)) if we can find a constant m and subspaces $U_n \subset Y_n$ such that (U_n, d) are ultrametric and $|U_n|^m \geq k_n$, for then $(n+1)^m \geq |U_n|^m \geq k_n$. This motivates the following discussion.

Let (A, d) be a finite metric space of cardinality k . Let $T(A)$ be the set of triangles in A and $T'(A)$ be the subset of those triangle violating condition 1. $|T(A)| = \binom{k}{3}$. Similarly consider (A_k, d) , a sequence of finite metric spaces of cardinality k , for arbitrarily large integers k .

Definition 7.2: (A_k, d) is almost ultrametric iff $\lim_{k \rightarrow \infty} \frac{|T'(A_k)|}{|T(A_k)|} = 0$
 (A, d) is q -almost ultrametric if $|T'(A)| \leq \binom{k}{3} k^{-q}$ for $q \geq 0$.

We will assume in the following Theorem that (A, d) is taken from one of cases (a),(b), or (c), with A n -dimensional.

Theorem 7.3: If (A, d) is q -almost ultrametric, then $|A| \leq \left(\frac{3\sqrt{3}}{2} n\right)^{\frac{2}{q}}$.

Proof: This is a corollary of a Theorem of J. Spencer[10] which states that the smallest set of triangles on k vertices such that there is no independent set of size l contains at least $\binom{k}{3}^3 \left(\frac{l-1}{2}\right)^{-2}$ triangles. (An independent set is defined as a set of vertices containing no triangles.) Thus A contains an independent set S of size r , so long as $\binom{k}{3} k^{-q} < \frac{4}{27} \frac{k^3}{(r-1)^2}$ which will be true for $r < \frac{2}{3\sqrt{3}} k^{\frac{3}{2}} + 1$. Thus there is an independent set of size $\frac{2}{3\sqrt{3}} k^{\frac{3}{2}} + 1$, and Theorem 1 establishes the bound on k .

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